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## RESEARCH ARTICLE

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### Key Points:

- Solidus and phase relations of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  were constrained using synchrotron Mössbauer spectroscopy and X-ray diffraction (XRD)
- Silicon significantly lowers the solidus temperatures of Fe-Ni alloys in both *fcc* and *hcp* structures
- Pixel-level XRD analysis enhances detection of liquid diffuse scattering and solidus identification

### Supporting Information:

Supporting Information may be found in the online version of this article.

### Correspondence to:

C. Zhou,  
[cijin@caltech.edu](mailto:cijin@caltech.edu)

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### Author Contributions:

**Conceptualization:** Cijin Zhou, Vasilije V. Dobrosavljevic, Jennifer M. Jackson

**Data curation:** Cijin Zhou, Vasilije V. Dobrosavljevic, Dongzhou Zhang, Jiyong Zhao, Thomas S. Toellner, Stella Chariton, Vitali B. Prakapenka, Jennifer M. Jackson

**Formal analysis:** Cijin Zhou

**Funding acquisition:** Jennifer M. Jackson

**Investigation:** Cijin Zhou, Vasilije V. Dobrosavljevic, Dongzhou Zhang, Wolfgang Sturhahn, Jennifer M. Jackson  
**Methodology:** Cijin Zhou, Vasilije V. Dobrosavljevic, Dongzhou Zhang, Wolfgang Sturhahn

**Resources:** Jiyong Zhao, Thomas S. Toellner, Stella Chariton, Vitali B. Prakapenka, Jennifer M. Jackson

**Software:** Wolfgang Sturhahn

**Supervision:** Vasilije V. Dobrosavljevic, Dongzhou Zhang, Jennifer M. Jackson

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## Solidus and Phase Relations of $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ at Earth's Core Conditions

Cijin Zhou<sup>1</sup> , Vasilije V. Dobrosavljevic<sup>2</sup> , Dongzhou Zhang<sup>3</sup> , Wolfgang Sturhahn<sup>1</sup> , Jiyong Zhao<sup>4</sup>, Thomas S. Toellner<sup>4</sup>, Stella Chariton<sup>3</sup> , Vitali B. Prakapenka<sup>3</sup> , and Jennifer M. Jackson<sup>1</sup> 

<sup>1</sup>Seismological Laboratory, California Institute of Technology, Pasadena, CA, USA, <sup>2</sup>Earth and Planets Laboratory, Carnegie Institution for Science, Washington, DC, USA, <sup>3</sup>Center for Advanced Radiation Sources, The University of Chicago, Chicago, IL, USA, <sup>4</sup>Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA

**Abstract** Determining the solidus of Fe-Ni-Si alloys at high pressure is important for constraining the thermal and compositional structure of Earth's core, where silicon is widely considered a major light element. However, large uncertainties remain due to methodological differences in melt-detection criteria and limited measurements in the hexagonal close-packed (*hcp*) phase field. In this study, we sampled the phase diagram of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  from 58 to 157 GPa and temperatures up to 3500 K using synchrotron Mössbauer spectroscopy (SMS) that monitors the atomic dynamics of iron nuclei, and synchrotron X-ray diffraction (XRD) to detect liquid diffuse scattering. SMS measurements constrained the solidus by tracking the collapse of hyperfine parameters across the solid–liquid boundary. Complemented by burst-heating XRD with pixel-level background analysis that enables robust identification of the appearance of liquid diffuse scattering, this dual-technique approach provides a precise determination of the solidus. Our results demonstrate that silicon significantly lowers the solidus temperatures of Fe-Ni alloys in both *fcc* and *hcp* structures, and the *hcp-fcc-liquid* quasi-triple point occurs at  $125 \pm 7$  GPa and  $2860 \pm 110$  K. At the highest solidus pressure of 150 GPa, we determine a low solidus temperature of  $3110 \pm 60$  K. This integrated framework enables a more precise determination of the solidus and provides broader insight into melting detection strategies relevant to Earth's deep interior.

**Plain Language Summary** The melting of core-forming Fe-Ni alloys is critical to understand the temperature of Earth's core. Silicon is believed to be one of the major light elements in the core, yet its effect on the solidus of Fe-Ni alloys at extreme pressures remains uncertain due to inconsistent melting criteria, varying experimental techniques, and lack of data. In this study, we conducted melting experiments on  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  up to 157 GPa and 3500 K using two different synchrotron-based techniques to track both changes in atomic dynamics and the first appearance of liquid signals. Our results reveal that adding 10 at.% silicon significantly lowers the solidus of  $\text{Fe}_{0.9}\text{Ni}_{0.1}$  across a wide range of pressures. More broadly, our work demonstrates a new strategy to detect melting under extreme conditions, which can be applied to other materials relevant to planetary interiors.

## 1. Introduction

Understanding the thermal and compositional structure of Earth's core is crucial for deciphering major geophysical phenomena, including the evolution of the core and the geodynamo (Davies et al., 2015; Nimmo, 2015; Wilson et al., 2025). Cosmochemical and seismological studies suggest that Earth's core is predominantly composed of iron with ~5 wt.% nickel, with lighter elements such as Si, O, C, and S incorporated (Hirose et al., 2013, 2021; McDonough & Sun, 1995; Nimmo, 2025). Among these, Si is commonly proposed as a major candidate light element as a consequence of the metal-silicate equilibrium during the core formation process (e.g., Hin et al., 2014; Ozawa et al., 2009; Shahar et al., 2009). Therefore, constraining the melting temperature in the Fe-Ni-Si system provides invaluable insights into the thermal state of Earth's core.

Despite the importance of constraining the melting temperature of core-forming materials, studies on high-pressure melting of Fe-Ni alloys remain rare and controversial. Persistent discrepancies among experimental techniques and melt-detection diagnostics have led to significant disparities in reported melting curves of these alloys (Fischer, 2016; Parisiades, 2021). In addition, while the influence of light elements on the melting temperature of Fe-Ni alloys has been recognized as important, it remains poorly explored. Previous studies have

**Validation:** Vasilije V. Dobrosavljevic, Wolfgang Sturhahn, Jennifer M. Jackson  
**Visualization:** Cijin Zhou  
**Writing – original draft:** Cijin Zhou  
**Writing – review & editing:** Cijin Zhou, Vasilije V. Dobrosavljevic, Dongzhou Zhang, Wolfgang Sturhahn, Jennifer M. Jackson

primarily focused on Fe-light element systems such as Fe-Si (Edmund et al., 2022; Ezenwa et al., 2024; Fischer et al., 2013; Ozawa et al., 2016) and Fe-C (Komabayashi et al., 2024; Lord et al., 2009; Mashino et al., 2019; Morard et al., 2017). However, the light element concentrations in these studies often exceed geochemical and geophysical estimates, and the investigated alloys frequently lack the hexagonal close-packed (*hcp*) crystal structure that is extensively suggested as the stable phase under Earth's core conditions (Kraus et al., 2022; Stixrude, 2012; Tateno et al., 2010).

In this study, we present a series of high  $P - T$  experiments on  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  up to 157 GPa and  $\sim 3500$  K, using a recently developed in situ dual-technique approach at the Advanced Photon Source (APS) that involves both synchrotron Mössbauer spectroscopy (SMS) and X-ray diffraction (XRD) (Dobrosavljevic et al., 2022, 2023). We conducted  $\sim 850$  Mössbauer measurements over eight SMS heating runs at beamline 3-ID-B to monitor the atomic dynamics of  $^{57}\text{Fe}$  nuclei across the solid-liquid phase boundary, and collected  $\sim 1200$  diffraction images over eleven XRD burst heating runs at beamline 13-ID-D to detect liquid diffuse scattering, constrain the *hcp-fcc* phase boundary and sample thermal pressure evolution, as well as monitor any carbon contamination during heating. At the highest pressures studied in our experiments, melting of *hcp*-structured  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  alloy is achieved. These characterizations enable us to constrain the *hcp-fcc-liquid* quasi-triple point and the solidus of *hcp*- $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ , providing a significant step toward a reliable melting curve for core-forming alloys under conditions relevant to Earth's core.

## 2. Experimental Methods

### 2.1. Sample Preparation

The sample material,  $^{57}\text{Fe}_{0.80(1)}\text{Ni}_{0.10(1)}\text{Si}_{0.10(1)}$ , was synthesized by arc-melting individual pieces of Ni, Si, and 95%-enriched  $^{57}\text{Fe}$ . The detailed synthesis procedure and sample characterization are described in Morrison et al. (2018). For simplicity, we refer to this composition as  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  throughout this paper. Samples from the same batch have been previously used to constrain the equation of state by XRD up to 175 GPa (Morrison et al., 2018), to determine thermoelasticity and sound velocities up to 86 GPa (Morrison et al., 2019), and to investigate the melting and phase diagram up to 82 GPa (Dobrosavljevic et al., 2022).

High pressure-temperature ( $P - T$ ) conditions were generated using laser-heated diamond anvil cells (DACs). Cubic boron nitride seats were placed on the downstream side of each DAC to maximize the accessible  $2\theta$  range for in situ XRD measurements. All DACs used rhenium (Re) gaskets with an initial thickness of 250  $\mu\text{m}$  which were pre-indented and drilled according to the target pressure range. A pair of diamond anvils with 300  $\mu\text{m}$  flat culets was used for experiments below 80 GPa, with the Re gasket pre-indented to 55  $\mu\text{m}$  and drilled with a 120  $\mu\text{m}$  hole using an electron discharge machine (EDM). The  $\sim 10$   $\mu\text{m}$ -thick  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  foil was sandwiched between dehydrated KCl flakes that served as both the pressure medium and thermal insulation. One ruby sphere was loaded away from the sample and used as the pressure marker during room-temperature compression. For experiments between 80 and 120 GPa, diamond anvils with 250  $\mu\text{m}$  culets beveled to 300  $\mu\text{m}$  were used with Re gaskets pre-indented to 35–40  $\mu\text{m}$  and EDM-drilled with 85  $\mu\text{m}$  holes, while maintaining the same KCl-sample-KCl configuration and ruby marker. Experiments greater than 120 GPa were conducted using diamond anvils with 150  $\mu\text{m}$  culets beveled to 300  $\mu\text{m}$ , with the Re gasket pre-indented to  $\sim 30$   $\mu\text{m}$  thick and drilled with a hole of 50  $\mu\text{m}$  using a laser drilling system. The sample foil was thinned down to  $\sim 7$   $\mu\text{m}$  to enhance thermal insulation within the small sample chamber, and no ruby was loaded.

After loading, each DAC was baked in a vacuum oven for 24 hr to minimize moisture and oxygen in the sample chamber and subsequently sealed. Each DAC was then compressed to its target pressure. All DACs were laser-annealed at around 1500 K prior to high-temperature measurements to relax deviatoric stress. For the  $>120$  GPa series, the first two runs were performed at the targeted room-temperature pressure and adequately annealed before experiments. This DAC was then further compressed for a final, highest pressure run ( $P_{300\text{K}} = 137$  GPa).

### 2.2. Experimental Procedures

#### 2.2.1. Synchrotron Mössbauer Spectroscopy

The atomic dynamics of the iron nuclei is used as a diagnostic of melting and is probed using the synchrotron Mössbauer spectroscopy (SMS) technique to detect the melting of Fe (Jackson et al., 2013),  $\text{Fe}_{0.9}\text{Ni}_{0.1}$  (D. Zhang et al., 2016),  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  (Dobrosavljevic et al., 2022) and FeO (Dobrosavljevic et al., 2023) to pressures of

82 GPa, 125 GPa, 73 GPa, and 59 GPa, respectively. The observed time-delayed signal is caused by coherent elastic scattering of synchrotron X-rays while traversing a sample containing solid bound  $^{57}\text{Fe}$  nuclei. The  $^{57}\text{Fe}$  nuclei are excited by incident x-rays and subsequently decay from the first excitation state, characterized by a transition energy of 14.4 keV and an excitation lifetime of 141 ns. This phenomenon is quantitatively described by the  $T$ -dependent Lamb–Mössbauer factor  $f_{LM} = e^{-k^2\langle u^2 \rangle}$ , where  $k$  is the wavenumber of the incident resonant x-rays, and  $\langle u^2 \rangle$  is the mean-square displacement of the  $^{57}\text{Fe}$  nuclei. Upon melting, as the mean-square displacement of the solid-bound nucleus becomes very large during the nuclear lifetime, the Lamb–Mössbauer factor consequently approaches zero.

SMS heating experiments are conducted at beamline 3-ID-B of the APS in top-up mode with 24 bunches that are separated by 153 ns. The incident X-ray beam is tuned to the 14.4 keV nuclear resonance of  $^{57}\text{Fe}$  with resolution of 1 meV using a silicon high-resolution monochromator (Toellner, 2000). The shape and full width at half maximum (FWHM,  $\sim 19 \times 30 \mu\text{m}^2$ ) of the X-ray beam are measured by knife-edge scans using tungsten rods before each melting run. Double-sided infrared (IR) laser heating (FWHM  $\sim 30 \times 30 \mu\text{m}^2$ ) is implemented using two continuous-wave fiber lasers. The sample is scanned in both  $x$  and  $y$  directions to map its topography and ensure alignment between the X-ray and IR laser focal areas. Alignment of the laser hotspot and the X-ray beam is then visually verified before and after each heating run using cameras, and any small misalignment in hotspot position arising from thermal drift of laser optics is monitored. In each heating run, the output laser powers are controlled by a computer acquisition sequence that features an incremental ramp of laser power, while collecting time-integrated Mössbauer signal intensity every 3 s. During each heating sequence, sample temperatures are monitored from both sides using a CCD spectrometer with the spectral fitting of thermal emission curves, while upstream and downstream X-ray intensities were simultaneously recorded by two ionization chambers. Changes in transmitted X-ray flux are used to estimate sample thinning during heating, which remain below 2% before the onset of melting. Pressures before SMS heating runs are determined using the offline Raman spectroscopy system at GSECARS of the APS. After SMS heating runs, we collected XRD patterns at each SMS heating spot at GSECARS' beamline 13-ID-D to assess carbon contamination as well as to constrain the post-heating sample pressures (Figures S1 and S2 in Supporting Information S1).

Each SMS heating run follows a standardized experimental sequence designed to ensure reproducibility. Prior to heating, a room-temperature time spectrum is collected. The heating spot is then heated at  $\sim 1,500$  K for approximately 5 min to anneal the sample heating location and adjust the laser power ratio such that the temperature readouts from both sides are balanced. A high-temperature time spectrum is obtained during the annealing and is analyzed to constrain a starting effective thickness of the sample heating location, which serves as a key parameter for the following fitting procedure. After each heating cycle, the lasers are quenched and a second room-temperature time spectrum is collected at the same location to assess potential changes in the sample. The total time for each heating run is around 3–5 min following the start of the acquisition sequence (See Table S1 in Supporting Information S1 for a summary of heating conditions for each SMS run).

We performed a total of eight SMS heating runs. Two of these runs exhibited carbon contamination, evidenced by the appearance of reflections that can be assigned to  $\text{Fe}_3\text{C}$  in their post-heating XRD patterns (Figure S2 in Supporting Information S1). In three additional runs, either the laser-heating spot was misaligned with the X-ray beam or the probed region did not reach melting, resulting in no clear loss of the SMS signal intensity at high temperature. These five runs were therefore excluded from further consideration, and the remaining three uncontaminated and well-aligned runs were used for analysis and discussion.

## 2.2.2. X-ray Diffraction

Synchrotron XRD is an in situ technique that is sensitive to atomic positions and capable of probing phase transitions under extreme conditions. The onset of melting in the sample is revealed by the appearance of liquid diffuse scattering, which originates from atomic disorder in the liquid state and can be superimposed on crystalline XRD patterns, accompanied by an increase in background intensity. XRD measurements additionally provide valuable information on the evolution of the long-range structural ordering that can be used to constrain the  $hcp$  –  $fcc$  phase boundary and monitor carbon contamination. Bragg reflections of  $fcc$  and  $hcp$  phases, as well as from B2-KCl, are fit to determine the unit-cell volumes at high temperature, from which the in situ pressures can be derived. These measurements allow quantification of the thermal pressure contributions within the sample chamber as a function of temperature. Thermal pressures are evaluated and applied as a correction to

the pressures used for SMS runs (see Section 2.4). In addition to the pressure determination, the evolution of integrated reflection intensities of *fcc* and *hcp* phases is monitored throughout heating, and used as a proxy for XRD melting detection.

XRD measurements are conducted at GSECARS' beamline 13-ID-D of the APS, using a Pilatus IM CdTe area detector and monochromatic incident X-rays of energy 37 keV ( $\lambda = 0.3344 \text{ \AA}$ ) with a focus spot size of  $\sim 3 \times 3 \mu\text{m}^2$  FWHM. A  $\text{LaB}_6$  standard material is used to calibrate the detector distance and diffraction geometry. The double-sided infrared laser heating system installed at beamline 13-ID-D produces a flat-top laser spot with a diameter  $\sim 10 \mu\text{m}$  (Prakapenka et al., 2008). Burst heating mode is used in all the XRD heating experiments to collect alternating pairs of high-temperature ("hot") and 300 K ("quenched") measurements with an exposure time of 1 s. In this mode, the sample is rapidly heated by short laser pulses and then quenched back to 300 K. This approach enables background updating using the corresponding quenched pattern as a reference for each high-temperature measurement (Dobrosavljevic et al., 2022). Burst heating also minimizes the sample's exposure to the laser beam, helping reduce chemical reactivity and diffusion during heating. Table S2 in Supporting Information S1 summarizes the heating conditions for each XRD run, including heating duration and explored temperature range. During heating, thermal emission spectra of the laser-heated area are recorded with a PIMAX-3 CCD detector (Princeton Instruments) and fitted to gray-body radiation curves using the software T-Rax (Prescher, 2016). Laser powers were increased and adjusted during each burst heating cycle to target higher temperatures while maintaining a balance of upstream and downstream temperatures.

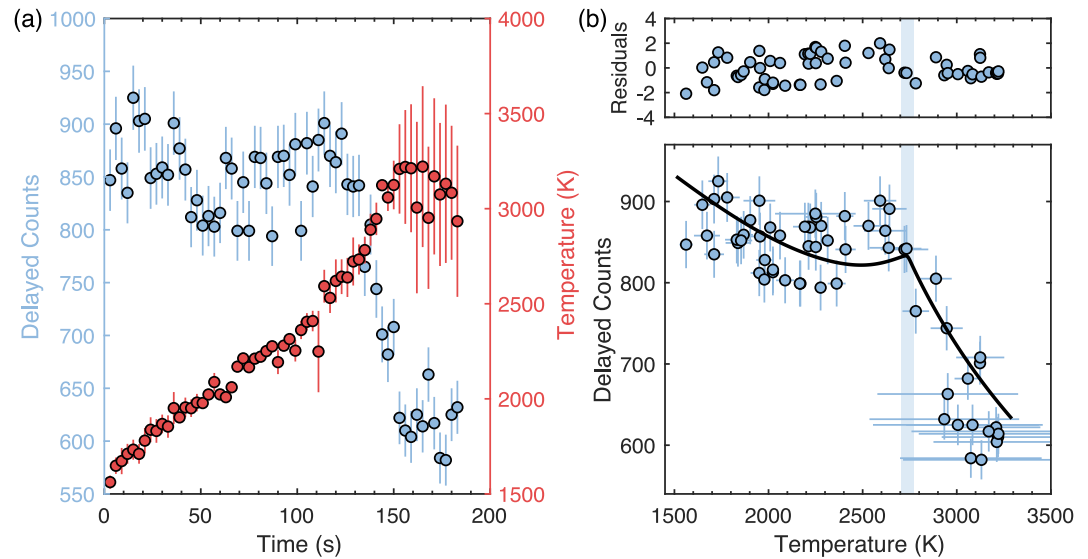
A total of eleven XRD burst-heating runs were conducted in this study. Four of these runs showed evidence of carbon contamination during heating, indicated by the appearance of  $\text{Fe}_3\text{C}$  diffraction peaks in XRD patterns (Figure S3 in Supporting Information S1), and were therefore excluded from further analysis. All subsequent analyses, including melting determination, thermal-pressure evaluation, and phase identification, are based on the remaining seven uncontaminated runs.

## 2.3. Detection of Solidus

### 2.3.1. Synchrotron Mössbauer Spectroscopy

Solidus temperatures of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  are determined using the time-domain SMS at pressures up to 111 GPa. The Mössbauer signal (time-integrated delayed counts) is caused by the coherent elastic scattering of synchrotron X-ray photons scattered in the forward direction that are delayed due to the nuclear excitation of  $^{57}\text{Fe}$ . The strength of the SMS signal, produced exclusively by the solid-bound  $^{57}\text{Fe}$  nuclei, is primarily determined by the effective thickness  $\eta$  of the sample, which is a dimensionless number and is proportional to the temperature-dependent Lamb-Mössbauer factor  $f_{LM}$  (Sturhahn, 2000). Upon melting, the measured Mössbauer signal drops precipitously (Figure 1a and 1b). This phenomenon has been used as a probe to detect melting (Dobrosavljevic et al., 2022; Dobrosavljevic et al., 2023; D. Zhang et al., 2016; Jackson et al., 2013). The solidus temperature of each SMS heating run is quantitatively determined by fitting the delayed counts - temperature profile with an experiment-specific scattering intensity model using the SIMX module in the software MINUTI 2.4beta5 (Sturhahn, 2025b), which models the sample effective thickness  $\eta$  and thus the measurable SMS signal intensity as a function of temperature.

Effective thickness  $\eta = f_{LM}\sigma\rho d$  is the dimensionless product of the numerical density of Fe nuclei ( $\rho$ ), the physical thickness of the sample ( $d$ ), the nuclear resonant cross-section ( $\sigma = 2.56 \times 10^{-22} \text{ m}^2$  for  $^{57}\text{Fe}$ ), and the Lamb-Mössbauer factor  $f_{LM}$ . SMS time spectra collected at  $\sim 1,500 \text{ K}$  during the annealing stage were analyzed using CONUSS software (Sturhahn, 2025a) to determine the effective thickness of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  at the start of each SMS heating run. Because no direct high-temperature XRD measurements were conducted at the same SMS heating location at beamline 3-ID-B, XRD patterns collected at  $\sim 1,500 \text{ K}$  on the same sample during XRD heating runs at beamline 13-ID-D are used to estimate sample density  $\rho$ , which was then used as an input parameter in determining  $\eta$ . The starting effective thickness of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  (derived from fitting the  $\sim 1,500 \text{ K}$  SMS time spectra), the time window used for signal integration, and the sizes and shapes of the X-ray beam and heating spot are provided as experiment-specific parameters to the SIMX module and summarized in Table S3 in Supporting Information S1. By incorporating experiment-specific inputs with an underlying physical model describing the temperature-dependent evolution of SMS signals, this approach yields a robust and quantitative framework for constraining the solidus temperature. The determined solidus temperatures along with the



**Figure 1.** (a) Typical synchrotron Mössbauer spectroscopy heating experiment showing the evolution of Mössbauer signal (delayed counts) during heating (run Y23CP4C,  $P_{300K} = 103$  GPa). Time-integrated delayed counts (blue, left axis) and temperature (red, right axis) were measured in 3 s intervals, with laser power incrementally increased between intervals. A sudden drop-off in delayed counts marks the onset of melting. (b) Corresponding fit to the delayed counts–temperature evolution using the SIMX module of the MINUTI software package (Sturhahn, 2025b). The solid black curve represents the best-fit model, and the blue shaded bar indicates the best-fit solidus temperature and uncertainty. Normalized residuals are plotted above the fit.

associated reduced  $\chi^2$  value from SIMX module are reported in Table 1 (see Figures S4–S6 in Supporting Information S1 for individual fitting results for each run).

### 2.3.2. X-ray Diffraction

Diffuse scattering is a characteristic of liquids and has been extensively used as a criterion to detect melting (e.g., Anzellini et al., 2013). However, the observation of such diffuse signals requires that the intensity must overcome a relatively large baseline background to be statistically detectable, and thus is challenging to identify solely from visual inspection of diffraction patterns. Dobrosavljevic et al. (2022) has introduced a background updating method for burst heating experiments. By normalizing each hot background intensity with its corresponding quenched background, the shape and intensity of the reference background are updated for each temperature step, and detection of the onset of diffuse scattering is enhanced.

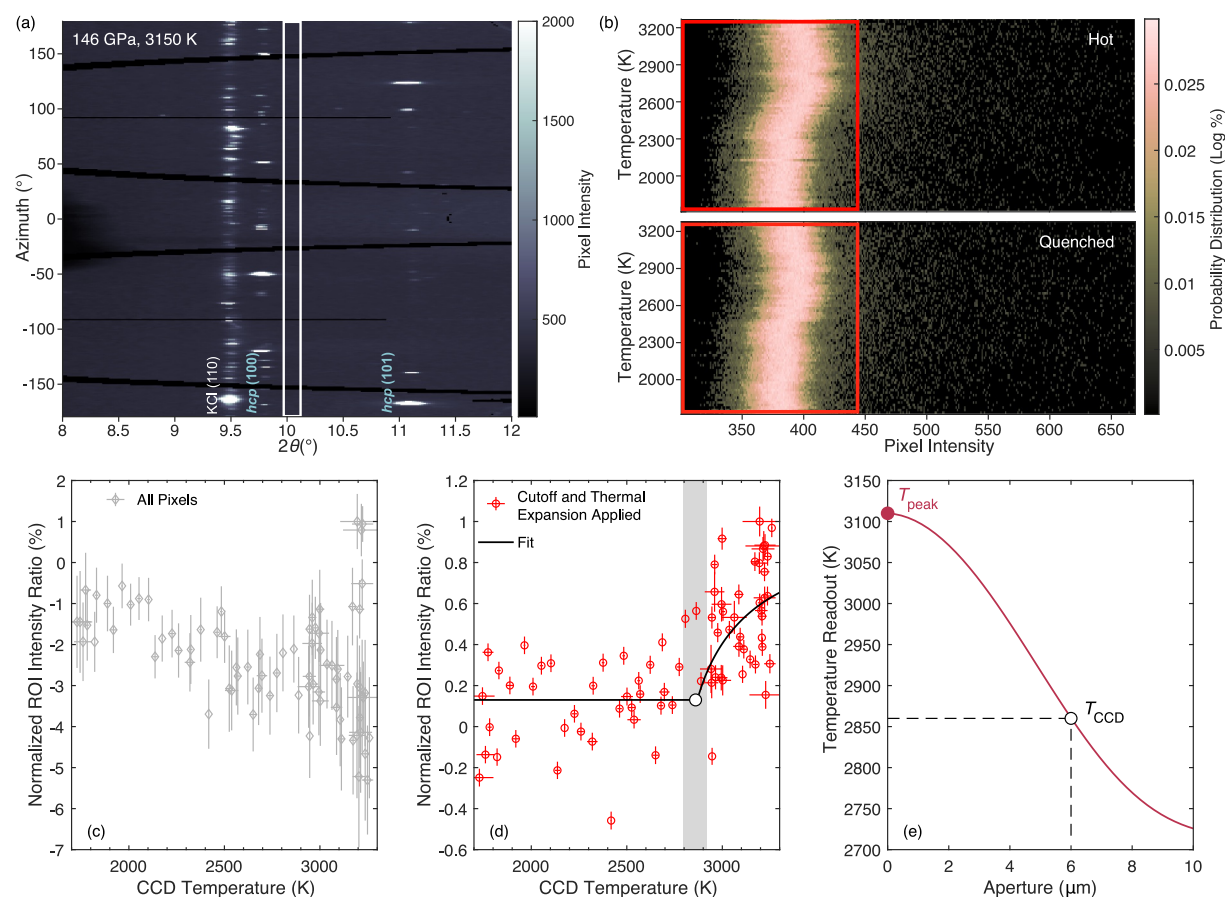
To further improve the sensitivity of melting detection and quantitatively track the development of liquid diffuse scattering with temperature under extreme conditions, we performed a pixel-level analysis of the XRD images using the SBCK module of MINUTI 2.4beta5 (Sturhahn, 2025b). Figure 2 illustrates the procedure using an example run Y23D8P2 ( $P_{300K} = 137$  GPa). A small region of interest (ROI, a  $2\theta$  range across all azimuthal angles, with the white box in Figure 2a as an example) was selected on the caked diffraction image to sample the background intensity adjacent to the major diffraction peak  $hcp(100)$  from  $Fe_{0.8}Ni_{0.1}Si_{0.1}$ , where the liquid diffuse scattering is expected to emerge most strongly. For each temperature step, the same analysis was repeated and the

box position was adjusted using a linear thermal-expansion to account for the gradual shift of the diffraction rings with increasing temperature. By analyzing the probability distributions of all selected pixel intensities at different temperatures (Figure 2b), we could distinguish between the consistent background and the erratic high-intensity pixels caused by instrumentation noise and/or the tails of Bragg peaks.

The core of our new approach involves applying a selective cutoff value to pixel intensity distributions, which is determined to ensure that the primary Gaussian population was captured while excluding the high-intensity skew.

**Table 1**  
Experimental Results and Solidus Temperatures of  $Fe_{0.8}Ni_{0.1}Si_{0.1}$   
Determined by Synchrotron Mössbauer Spectroscopy

| Run      | $P_{300K}$ (GPa) | $P_{solidus}$ (GPa) | $T_{solidus}$ (K) | SIMX reduced $\chi^2$ |
|----------|------------------|---------------------|-------------------|-----------------------|
| Y23D1S3  | 58(1)            | 65(4)               | 2,470(40)         | 2.50(19)              |
| Y22CP4S2 | 88(2)            | 96(5)               | 2,690(20)         | 1.94(14)              |
| Y23CP4C  | 103(3)           | 111(5)              | 2,740(30)         | 1.30(15)              |



**Figure 2.** Example pixel-intensity analysis used to extract background intensity for run Y23D8P2 ( $P_{300K} = 137$  GPa), performed using the SBCK module of the MINUTI software package (Sturhahn, 2025b). (a) Representative X-ray diffraction caked image at  $\sim 146$  GPa and 3,150 K. The white box marks the region of interest (ROI) near the hcp (100) reflection used for background analysis. For each temperature, the same procedure was applied, with the ROI position adjusted using a linear thermal expansion to account for the shift of diffraction peaks with increasing temperature. (b) Pixel-intensity distributions from the selected ROIs at different temperatures. The red box indicates the pixel-intensity range selected for cutoff filtering. (c) Temperature dependence of normalized hot-background intensity obtained using all pixels from panel (b), following the background-updating procedure of Dobrosavljevic et al. (2022). (d) Same analysis as in panel (c), but after applying the pixel-intensity cutoff shown in panel (b). Excluding high-intensity outliers suppresses background fluctuations and enhances the diffuse-scattering signal associated with melting. The black solid curve shows the fit to the processed background intensities using the SIMX module of MINUTI (Sturhahn, 2025b). (e) Conversion from the CCD-measured average temperature ( $T_{CCD}$ ; open circle from panel (d)) to the corresponding peak hotspot temperature ( $T_{peak}$ ). The conversion is based on the spatial profile of the laser hotspot and the spectrograph aperture (6  $\mu\text{m}$ ). The final reported solidus temperature corresponds to  $T_{peak}$  (red solid circle at zero aperture).

As shown in Figure 2b, the cutoff value was manually optimized for both hot and quenched frames to ensure that the Gaussian portion of the pixel intensity distributions was not truncated while excluding outlier pixels. By including only pixels within this defined range (red boxes in Figure 2b), we prevent background quantification from being biased by high-intensity pixels. This filtering ensures that the resulting background intensity accurately reflects the sample's state rather than fluctuations of pixel intensities. Sensitivity analysis indicates that the results are robust against minor variations in the exact placement of the cutoff. Although shifting the cutoff value slightly changes the absolute signal-to-noise ratio, the overall shape of the intensity trend remains consistent (Figures S7a–S7c in Supporting Information S1). However, if the cutoff is set too low such that the main Gaussian distribution is not fully captured, the intensity trend becomes scattered, losing the clear increase at high temperature (Figure S7d in Supporting Information S1). This confirms that the increase in normalized ROI intensity is a true reflection of the structural phase change in the sample rather than an artifact of the data processing parameters.

Figures 2c and 2d illustrate the advantage of the cutoff-filtered approach over the standard all-pixel integration. Both datasets were normalized (hot/quenched) using the same background updating procedure suggested in Dobrosavljevic et al. (2022). By excluding high-intensity outliers, the pixel-value cutoff effectively suppresses

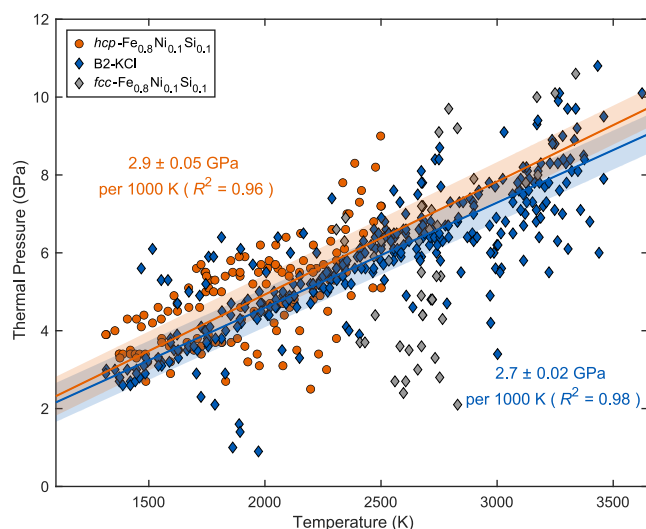
**Table 2**  
*Experimental Results and Solidus Temperatures of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  Determined by X-ray Diffraction*

| Run       | $P_{300\text{K}}$<br>(GPa) | $P_{\text{hcp-fcc}}$<br>(GPa) | $T_{\text{hcp-fcc}}$<br>(K) | $P_{\text{solidus}}$<br>(GPa) | $T_{\text{CCD}}$<br>(K) | $T_{\text{solidus}}$<br>(K) | SIMX<br>Goodness of fit |
|-----------|----------------------------|-------------------------------|-----------------------------|-------------------------------|-------------------------|-----------------------------|-------------------------|
| Y23D1S4   | 70(1)                      | 74(2)                         | 2,280(60)                   | 75(2)                         | 2,420(220)              | 2,610(220)                  | 4.12(43)                |
| Y23D1S5   | 68(1)                      | 72(2)                         | 2,240(75)                   | 74(2)                         | 2,440(70)               | 2,640(70)                   | 7.31(46)                |
| Y22CP4S3  | 90(2)                      | 97(3)                         | 2,580(75)                   | 100(3)                        | 2,580(60)               | 2,800(60)                   | 6.37(47)                |
| Y22CP4S4  | 90(2)                      | 95(3)                         | 2,450(100)                  | 96(4)                         | 2,645(50)               | 2,870(50)                   | 2.82(29)                |
| Y22D8P1S1 | 130(3)                     |                               |                             | 137(4)                        | 2,710(60)               | 2,940(60)                   | 47.10(89)               |
| Y23D8P1S2 | 132(2)                     |                               |                             | 139(3)                        | 2,675(80)               | 2,900(80)                   | 48.98(78)               |
| Y23D8P2   | 137(3)                     |                               |                             | 150(6)                        | 2,860(60)               | 3,110(60)                   | 24.04(57)               |

fluctuations and isolates the subtle rise in background intensity, which is associated with diffuse scattering from melts. The refined background intensity evolution reveals a distinct, statistically significant discontinuity at the onset of melting. For runs Y22CP4S4 and Y23D1S4, recrystallization prior to the *hcp* – *fcc* phase transition led to enhanced pixel-level intensity heterogeneity, and a more restrictive pixel-value cutoff was therefore adopted within the same cutoff-based framework to mitigate this effect.

Representative integrated XRD patterns collected at temperatures below, near, and above the constrained solidus temperature are shown in Figure S8 in Supporting Information S1. Subtle diffuse scattering is observed in the background region of patterns collected near the inferred solidus temperature, while diffuse scattering becomes more pronounced at temperatures above the solidus. However, the initial appearance of diffuse scattering remains difficult to identify confidently by visual inspection alone, particularly near the onset of melting where the liquid signal is very weak. These observations highlight the advantage of the quantitative pixel-level background analysis employed here, which tracks systematic changes in pixel intensity distributions within selected background regions to more robustly constrain the onset of melting.

For each burst heating sequence, the solidus temperature is determined by fitting the temperature dependence of the normalized background using the SIMX module of MINUTI 2.4beta5 (Sturhahn, 2025b). The fitting procedure was performed without imposing prior constraints on the solidus temperature. The model accounts for both the laser-heating hotspot profile and the X-ray beam profile at beamline 13-ID-D as input parameters to simulate the spatial temperature distribution within the probed area. Because the exact laser hotspot profile was not directly measured in XRD experiments, a Gaussian intensity distribution with a FWHM of 10  $\mu\text{m}$  was assumed as a reasonable approximation based on typical laser-heating conditions. In laser-heating experiments, the temperature measured by the spectrograph represents an average value over the collection region rather than the true peak temperature. For the laser heating configuration at beamline 13-ID-D, the spectrograph monitored an approximately 6  $\mu\text{m}$  diameter region at the center of the laser hotspot, providing an intensity-weighted mean temperature within the probed area. However, melting typically begins at the hottest region of the spot, corresponding to the peak temperature across the spatial temperature gradient. The SIMX module in MINUTI accounts for this effect by converting the CCD-measured average temperature to the corresponding peak temperature, based on the input spatial profile of the laser hotspot and the spectrograph aperture (Figure 2e). To assess the sensitivity of the inferred melting temperatures to the assumed spatial temperature distribution, additional simulations were performed using alternative profiles, including sharper and flatter temperature distributions (Figure S9 in Supporting Information S1). These tests indicate that reasonable variations in the assumed temperature profile do not significantly affect the inferred peak melting temperatures, with resulting  $T_{\text{peak}}$  values remaining within mutual uncertainties. This allows a more accurate determination of the solidus temperature that is physically representative of the onset of melting, and fitting results of seven XRD heating runs are summarized in Table 2 (see Figures S10–S16 in Supporting Information S1 for individual fitting results for each run). The same framework is also applied in our SMS analysis (Section 2.3.1); however, for SMS experiments, the laser hotspot ( $\sim 30 \mu\text{m}$  in diameter) is much larger than the spectrograph-monitored area ( $\sim 5 \mu\text{m}$  in diameter), the CCD-measured temperature and the peak temperature are nearly identical in that case, and the conversion is negligible considering uncertainties.



**Figure 3.** Summary of thermal pressure data derived from all X-ray diffraction measurements in this study. Thermal pressure for each measurement was calculated as the difference between the in situ high-temperature pressure and its corresponding quenched pressure. Linear fits of thermal pressure slopes (solid lines) for  $hcp\text{-Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  (orange color;  $2.9 \pm 0.5$  GPa per 1,000 K) and B2-KCl (blue color;  $2.7 \pm 0.2$  GPa per 1,000 K) show excellent agreement.

sample pressures reported in this study correspond to those calculated from the thermal EOS of  $hcp\text{-Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ .

We calculate thermal pressures for  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  and KCl in each pair of burst heating as the difference between each hot pressure and its corresponding quenched pressure. Reflections of  $fcc$  phase are relatively weak in runs below the quasi-triple point, resulting in large uncertainties of  $fcc$  volumes and very scattered thermal pressures of the  $fcc$  phase. We note that the larger scatter of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  thermal pressures at  $T > 2500$  K is caused by the  $hcp\text{-}fcc$  phase transitions and recrystallization. To present a thermal pressure model with high statistical quality, we fit all  $hcp\text{-Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  thermal pressures at  $T < 2500$  K and KCl thermal pressures throughout the measured temperature range. We note that the sample in the highest-pressure run (Y23D8P2,  $P_{300\text{K}} = 137$  GPa) was not adequately annealed before heating, and we therefore excluded this dataset from the thermal-pressure model to avoid the effects of residual stress. We find a good agreement between the two materials: a linear fit to all sample thermal pressures constrains a slope of  $2.9 \pm 0.5$  GPa per 1000 K, which is consistent with the linear fit to all KCl thermal pressures ( $2.7 \pm 0.2$  GPa per 1000 K) as shown in Figure 3. We therefore report a thermal pressure model of  $2.8 \pm 0.2$  GPa per 1000 K. This result is in excellent agreement with the model reported by Dobrosavljevic et al. (2022) (2.9 GPa per 1000 K) for  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  loaded in a KCl medium. This thermal pressure model is applied to calibrate pressures in each SMS heating run, using 300 K pressures constrained from post XRD measurements on each SMS heating location conducted at beamline 13-ID-D, and an additional melting pressure uncertainty of 3 GPa. This added uncertainty accounts for uncertainties in the assumed KCl temperatures, while preserving agreement with previously published in situ measurements on Fe in a KCl pressure medium (Sinmyo et al., 2019), as shown in Figure S17 in Supporting Information S1.

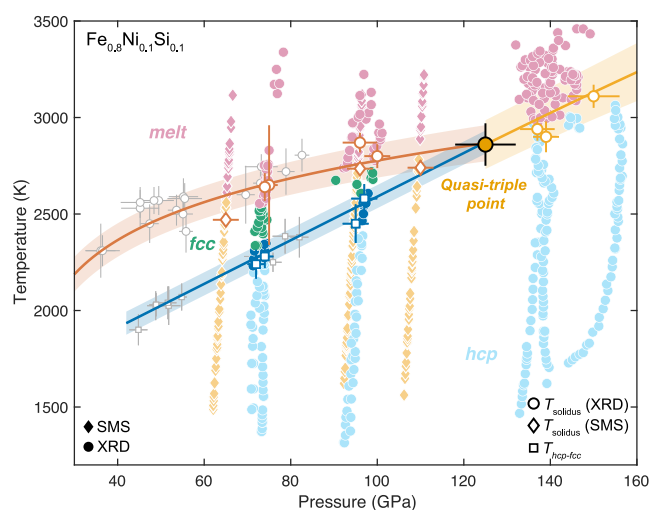
### 3. Results and Discussions

#### 3.1. Phase Relations and Solidus of $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$

XRD patterns collected during heating provide direct constraints on the crystal structures of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  at each  $P - T$  condition. Within the investigated  $P - T$  range, we determined that  $hcp$  and  $fcc$  are the only structures observed. The  $hcp - fcc$  transition temperature was primarily constrained by the  $fcc$ -in temperature because the  $hcp$  peak intensities were highly scattered (as discussed in Section 3.3), estimated at the point where  $fcc$  reflections reached about 20% of their maximum intensity. The phase boundary between  $hcp$  and  $fcc$  was

#### 2.4. Thermal Pressure Model and Sample Pressure Determination

A total of  $\sim 820$  XRD patterns from seven separate burst-heating runs were analyzed by full-profile refinement in GSAS-II (Toby & Von Dreele, 2013) over a pressure range of 71–157 GPa. In-situ pressures were determined from refined unit-cell volumes using previously published thermal equations of state (EOS) (Table S4 in Supporting Information S1). For the B2-KCl pressure medium, we used the thermal EOS of Tateno et al. (2019), assuming a KCl temperature equal to the average surface temperature of the laser-heated sample. This assumption follows Dobrosavljevic et al. (2022) and represents an upper-bound estimate of the KCl temperature within the sample chamber. As a lower-bound estimate, we also evaluated KCl thermal pressures assuming a temperature equal to the average of the sample surface temperature and 300 K (Campbell et al., 2009), as shown in Figure S17 in Supporting Information S1. Sample pressures were calculated using the EOS framework of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  for both  $hcp$  and  $fcc$  phases as described by Dobrosavljevic et al. (2022). For the  $hcp$  phase, we adopted the bulk modulus ( $K_{T0}$ ) and its pressure derivative ( $K'_{T0}$ ) from Komabayashi et al. (2019), using the model appropriate for solid pressure media, with thermal parameters adopted from Morrison et al. (2019). Due to the absence of high-fidelity  $P - T - V$  data for the  $fcc$  phase, we followed the same methodology of Komabayashi (2014), assuming identical  $K_{T0}$  and  $K'_{T0}$  to those of the  $hcp$  phase, and adjusting the  $V_0$  using the  $hcp/fcc$   $V_0$  ratio for pure Fe. Thermal parameters of the  $fcc$  phase are determined by Dobrosavljevic et al. (2022) based on refitting the  $fcc\text{-Fe}$  data set compiled by Komabayashi (2014). Unless otherwise noted,



**Figure 4.** Phase relations and pressure–temperature conditions of all validated melting experiments conducted in this study. Diamonds represent synchrotron Mössbauer spectroscopy measurements and circles represent X-ray diffraction heating runs without carbon contamination. Results from Dobrosavljevic et al. (2022) are included for phase boundary determination and are plotted as open circles for melting temperatures  $T_{\text{melt}}$ , and open squares for the  $hcp - fcc$  transition temperatures  $T_{hcp-fcc}$ . Solid phase boundaries determined in this study are shown as colored lines: blue for the  $hcp - fcc$  boundary, orange for the  $fcc$  solidus, and yellow for the  $hcp$  solidus.

resulting in the orange melting curve shown in Figure 4. The intersection of  $hcp - fcc$  boundary and  $fcc$ -solidus curve is calculated to constrain the location of the  $hcp - fcc - liquid$  quasi-triple point at  $125 \pm 7$  GPa and  $2860 \pm 110$  K.

Three XRD burst heating measurements Y22D8P1S1 ( $P_{300K} = 130$  GPa), Y23D8P1S2 ( $P_{300K} = 132$  GPa), and Y23D8P2 ( $P_{300K} = 137$  GPa) show clear characteristic fingerprints of solely  $hcp$ -structured  $Fe_{0.8}Ni_{0.1}Si_{0.1}$  before and upon melting. No  $fcc$  reflections were detected below the temperatures corresponding to the onset of diffuse scattering. At temperatures exceeding 3200 K across these three runs,  $fcc$  (111) and/or (200) reflections occasionally appeared in the collected XRD patterns, but only at substantially higher temperatures than the inferred melting temperature from diffuse scattering and thus beyond the solidus. The appearance of these  $fcc$  peaks at extreme temperatures is attributed to localized recrystallization in the colder regions of the volume probed by X-rays, likely caused by axial pressure and temperature gradients in the sample (Sinmyo et al., 2019). Consistent with this interpretation, pressures calculated from the thermal EOS of  $fcc$ - $Fe_{0.8}Ni_{0.1}Si_{0.1}$  using volumes from these reflections are  $\sim 5$ – $10$  GPa lower than the corresponding KCl pressures and  $hcp$ - $Fe_{0.8}Ni_{0.1}Si_{0.1}$  pressures at the same temperatures. Because these solidus points occur at higher pressures than the quasi-triple point, they are interpreted as representing the onset of melting of  $hcp$ - $Fe_{0.8}Ni_{0.1}Si_{0.1}$ .

Although the limited number of high-pressure  $hcp$  data points prevents a robust constraint of the solidus slope, in an effort to parameterize the solidus of  $hcp$ - $Fe_{0.8}Ni_{0.1}Si_{0.1}$  using data we collected at pressures relevant to Earth's core, here we apply the Simon–Glatzel equation and the quasi-triple point determined earlier as the reference point ( $T_{m0}, P_{m0}$ ), while  $x$  and  $y$  are estimated from the phonon density-of-states of  $hcp$ -Fe measured by nuclear resonant inelastic X-ray scattering (Murphy et al., 2011,  $x = 167 \pm 20$  GPa,  $y = 0.64 \pm 0.08$ ), with a reasonable assumption that the vibrational properties of  $hcp$ -Fe and  $hcp$ - $Fe_{0.8}Ni_{0.1}Si_{0.1}$  are similar (Morrison et al., 2019) (Figure 4, shown as the yellow curve).

### 3.2. Comparison With SMS Studies

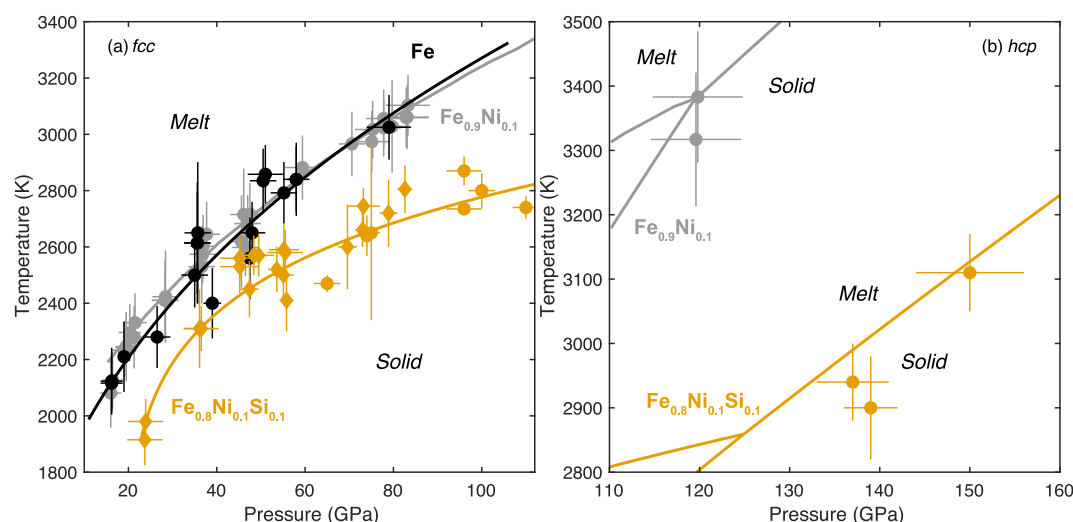
We first compare our results with previous studies on Fe and Fe alloys that employed the same SMS diagnostic method for melt detection, including those by Jackson et al. (2013), D. Zhang et al. (2016), and Dobrosavljevic et al. (2022). Each study was conducted at beamline 3-ID-B of the APS with nearly identical experimental setup.

determined by combining the results from this study (Table 2) with those of Dobrosavljevic et al. (2022) obtained on the same sample composition. The linear regression of the combined dataset yields a slope of  $11.1 \pm 0.6$  K/GPa and 0 GPa intercept of  $1460 \pm 40$  K ( $R^2 = 0.97$ ), in excellent agreement with the previously reported  $hcp - fcc$  phase boundary in Dobrosavljevic et al. (2022) (slope of  $11.6 \pm 0.9$  K/GPa and 0 GPa intercept  $1430 \pm 55$  K, shown in Figure 4 as the blue line). We note that while the 0 GPa intercept is reported here for the linear fit, the  $hcp - fcc$  boundary does not physically extend to ambient pressure (Witusiewicz et al., 2023).

Solidus temperatures of  $Fe_{0.8}Ni_{0.1}Si_{0.1}$  were constrained from SMS and XRD measurements up to 157 GPa. Within the investigated pressure range, melting below 120 GPa occurs in the  $fcc$  phase field, as indicated by the  $hcp - fcc$  phase transition in XRD patterns. The pressure dependence of the  $fcc$  solidus was parameterized using the empirical Simon–Glatzel equation (Simon & Glatzel, 1929):

$$T_m = T_0 \left( \frac{P_m - P_0}{x} + 1 \right)^y \quad (1)$$

where  $T_m$  is the solidus temperature at pressure  $P_m$ ,  $T_0$  is the melting temperature at a reference pressure  $P_0$ , and  $x$  and  $y$  are adjustable material-specific parameters. To ensure consistent coverage across the  $fcc$  stability field, the fitting was performed by combining the present data from this study with the dataset of Dobrosavljevic et al. (2022). We find best-fit values  $T_0 = 1,975(100)$  K,  $P_0 = 23.7(25)$  GPa,  $x = 4.3(27)$  GPa, and  $y = 0.12(2)$ ,



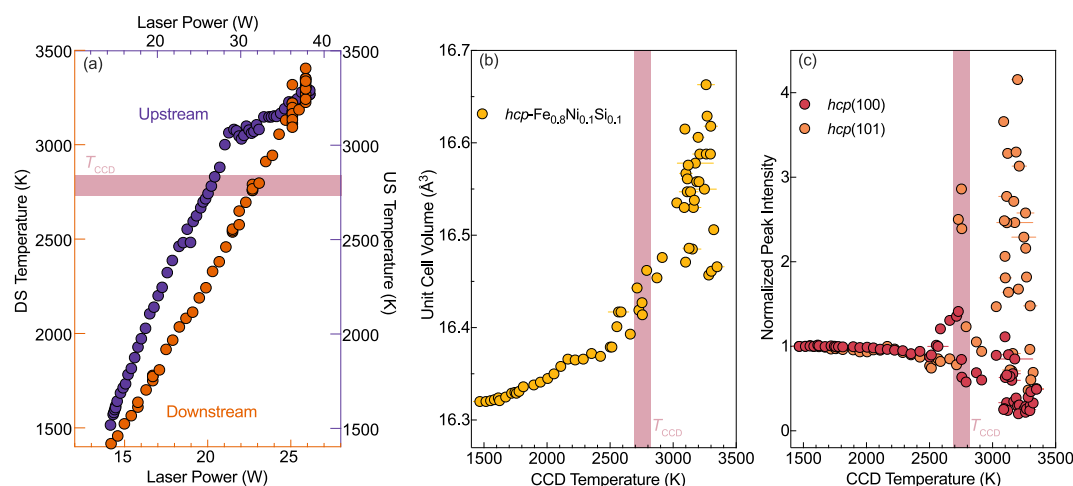
**Figure 5.** (a) Solidus curves of *fcc*-structured Fe and Fe alloys using the synchrotron Mössbauer spectroscopy (SMS) diagnostic method for melt detection. Orange curve represents the solidus of Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub>, determined using results from both this study (solid circle) and Dobrosavljevic et al. (2022) (solid diamond). Updated melting curves for *fcc*-Fe (solid black curve) and *fcc*-Fe<sub>0.9</sub>Ni<sub>0.1</sub> (solid gray curve) are adopted from Dobrosavljevic et al. (2022) based on SMS data from Jackson et al. (2013) and D. Zhang et al. (2016). (b) Solidus temperatures of *hcp*-Fe<sub>0.9</sub>Ni<sub>0.1</sub> (gray; D. Zhang et al., 2016) and *hcp*-Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub> (orange; this study).

Samples were prepared in the same KCl–sample–KCl configuration, laser-heated using the same double-sided system, and subjected to the same heating sequence and measurement procedure. The data analysis followed the same workflow, in which all experiment-specific parameters were incorporated into the SIMX module of MINUTI. The shared experimental and analytical design therefore allows a systematic and internally consistent comparison of the melt detection across compositions. Additionally, the solidus of *fcc*-Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub> determined in this study shows good agreement with melting temperatures reported by Dobrosavljevic et al. (2022) on the same sample alloy using the similar in situ dual-technique approach, confirming the repeatability and reproducibility of combining SMS and XRD techniques in investigations of melting.

For direct comparison, we adopt the updated melting curves for Fe (Jackson et al., 2013; D. Zhang et al., 2016) and Fe<sub>0.9</sub>Ni<sub>0.1</sub> (D. Zhang et al., 2016) as recalculated by Dobrosavljevic et al. (2022) using their reported thermal pressure model, which agrees very closely with the model independently constrained in this study, such that recalculation using our model would yield indistinguishable solidus curves. The updated results are plotted together in Figure 5a, where the *fcc* solidus points from all four studies define broadly similar trends with pressure. Across the entire pressure range investigated, the solidus of Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub> (this study; Dobrosavljevic et al., 2022) is significantly lower than those of Fe (Jackson et al., 2013) and Fe<sub>0.9</sub>Ni<sub>0.1</sub> (D. Zhang et al., 2016). This decrease with the addition of Si highlights the pronounced influence of light elements in lowering the melting temperature of Fe alloys at high pressures, indicating that the observed differences among datasets primarily reflect composition rather than methodological discrepancies. Figure 5b compares the solidus of *hcp*-Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub> reported in this study with that of *hcp*-Fe<sub>0.9</sub>Ni<sub>0.1</sub> reported by D. Zhang et al. (2016). The solidus temperatures of Fe<sub>0.8</sub>Ni<sub>0.1</sub>Si<sub>0.1</sub> are significantly lower than those of Fe<sub>0.9</sub>Ni<sub>0.1</sub> measured at lower pressures, demonstrating that the addition of 10 at.% silicon markedly reduces the melting temperature of Fe–Ni alloys at core pressures. Although the limited number of high-pressure data points prevents constraining the solidus slope, the observed solidus temperature depression provides strong evidence for the compositional effect of Si on melting in the *hcp* stability field.

### 3.3. Proxies for the Detection of Melting

We also investigate other commonly used proxies for melting detection in XRD studies. Many previous experimental studies have observed the appearance of a temperature plateau during laser heating (e.g., Lord et al., 2010) and attributed it to melting. In run Y22D8P1S1 ( $P_{300K} = 130$  GPa, Figure 6a), we observe a similar flattening or slope change with increasing laser power, and the onset of this behavior is above the solidus

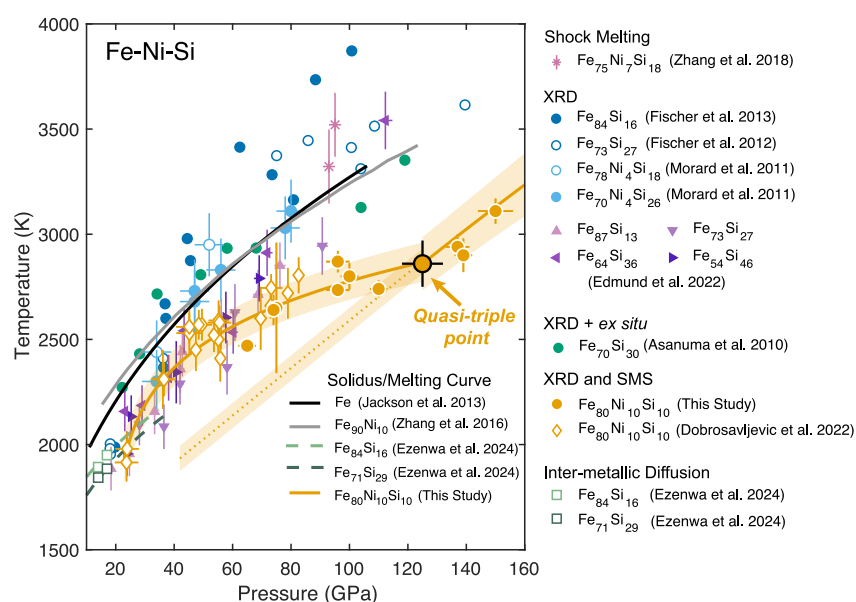


**Figure 6.** Run Y22D8P1S1 ( $P_{300\text{K}} = 130$  GPa) showing: (a) changes in sample temperature as a function of laser power output; (b) the unit-cell volume changes; and (c) the intensity changes of (100) and (101) peaks in  $hcp\text{-Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  with increasing temperature. Peak intensities are integrated and normalized by the starting intensity. Shaded bars represent the CCD-measured solidus temperature ( $T_{\text{CCD}}$ ) determined by fitting the temperature dependence of the normalized background with the SIMX module of the MINUTI software package (Sturhahn, 2025b) (see Section 2.3.2 for more details).

temperature determined by the onset of the diffuse scattering. In contrast, the downstream temperature increases smoothly. In Figure S18 in Supporting Information S1 we show the temperature–laser power profiles for an additional XRD run (Y23D1S4,  $P_{300\text{K}} = 70$  GPa) and an SMS run (Y23CP4C,  $P_{300\text{K}} = 103$  GPa). In run Y23D1S4, temperatures on both sides increase steadily before an abrupt jump with variable slopes. In run Y23CP4C, the downstream side generally shows a monotonic increase in temperature, whereas the upstream side gradually increases to a peak and then decreases toward the solidus. Although a subtle change in slope near the solidus may be present in some cases, it is difficult to identify without prior knowledge of the solidus temperature location. We therefore conclude that discontinuities in sample temperature as a function of laser power cannot be used as a reliable proxy for the onset of melting in this study.

We further examined the evolution of the sample volume, which has been proposed as a melting proxy for Fe based on the occurrence of a volume plateau (Anzellini et al., 2013). In our experiments on  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ , the evolution of unit-cell volume in all XRD burst heating runs shows large fluctuations with increasing temperature rather than a clear plateau upon melting. In run Y23D8P1S1 ( $P_{300\text{K}} = 130$  GPa, Figure 6b) exhibits scattering in the sample unit-cell volume as low as  $\sim 200$  K prior to the onset of melting. In contrast, Y23D8P2 ( $P_{300\text{K}} = 137$  GPa, Figure S10 in Supporting Information S1) and Y23D8P1S2 ( $P_{300\text{K}} = 132$  GPa, Figure S11 in Supporting Information S1), the sample unit-cell volumes increase abruptly upon melting, followed by large fluctuations and significant scattering at higher temperatures. Even more divergent behaviors were observed in other runs (Figures S13–S16 in Supporting Information S1). We interpret these variations as a consequence of the radial and axial  $P - T$  gradients within the X-ray probed volume. Once the solidus is crossed, the diffraction signal represents the residual solid in the cooler and lower-pressure regions, while the molten portion contributes only to the diffuse background. Collectively, these results demonstrate that unit-cell volume evolution is not a robust or reproducible indicator for the solidus of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ .

Discontinuities in diffraction peak intensity as a function of temperature have been proposed as another criterion of melting (e.g., Fu & Hirose, 2024; Kusakabe et al., 2019). In our burst-heating runs, however, the intensities of  $hcp(100)$  and  $(101)$  do not show a systematic decrease above the solidus; instead, they vary irregularly with large scatter. This behavior is exemplified by run Y22D8P1S1 ( $P_{300\text{K}} = 130$  GPa, Figure 6b). In this case, the intensity of  $hcp(100)$  begins to increase  $\sim 200$  K below the solidus, then transitions to a generally decreasing trend. In contrast, the  $hcp(101)$  reflection shows an abrupt intensity increase near the solidus, followed by a drop and then a fluctuation above 3,000 K. The complicated and variable behavior is also observed across all heating runs (Figures S10–S16 in Supporting Information S1). We attribute these variations again to the radial and axial  $P - T$  gradients within the X-ray probed volume. When approaching melting, the diffraction signal arises from residual solid in cooler and lower-pressure regions. This remaining solid undergoes grain growth and



**Figure 7.** Summary of melting relations in the Fe–Ni–Si system from this and previous studies. Orange symbols represent Fe<sub>80</sub>Ni<sub>10</sub>Si<sub>10</sub>, with solid circles showing solidus temperatures determined in this study and solid diamonds representing measurements from Dobrosavljevic et al. (2022). The solid orange curves correspond to the fitted solidus boundaries for the *fcc* and *hcp* phases based on Simon–Glatzel equation fitting. Solid black and gray curves are synchrotron Mössbauer spectroscopy melting curves for *fcc*-Fe (Jackson et al., 2013; D. Zhang et al., 2016) and *fcc*-Fe<sub>90</sub>Ni<sub>10</sub> (D. Zhang et al., 2016), respectively. Melting temperatures of Fe(–Ni)–Si from earlier studies using X-ray diffraction without burst heating and background updating are plotted as reported: dark blue solid circles, Fe<sub>84</sub>Si<sub>16</sub> (Fischer et al., 2013); dark blue open circles, Fe<sub>73</sub>Si<sub>27</sub> (Fischer et al., 2012); solid green circles, Fe<sub>70</sub>Si<sub>30</sub> (Asanuma et al., 2010); light blue open circles, Fe<sub>78</sub>Ni<sub>4</sub>Si<sub>18</sub> (Morard et al., 2011); light blue solid circles, Fe<sub>70</sub>Ni<sub>4</sub>Si<sub>26</sub> (Morard et al., 2011). Data from Edmund et al. (2022) are plotted as purple triangles with different orientations corresponding to different compositions: upward triangles, Fe<sub>87</sub>Si<sub>13</sub>; downward triangles, Fe<sub>73</sub>Si<sub>27</sub>; leftward triangles, Fe<sub>64</sub>Si<sub>36</sub>; and rightward triangles, Fe<sub>55</sub>Si<sub>45</sub>. Data from (Ezenwa et al., 2024) are plotted as open green squares (Fe<sub>84</sub>Si<sub>16</sub>) and open dark-green squares (Fe<sub>71</sub>Si<sub>29</sub>); the corresponding dashed curves represent extrapolated solidus relations based on low-pressure inter-metallic diffusion experiments constrained up to 17 GPa. Shock melting of Fe<sub>75</sub>Ni<sub>7</sub>Si<sub>18</sub> is shown in pink stars (Y. Zhang et al., 2018).

recrystallization, and both its fraction and crystallographic orientation evolve with increasing temperature. As a result, peak intensities fluctuate irregularly rather than displaying the sharp weakening expected for complete melting. The raw diffraction images further support this interpretation (Figures S19 in Supporting Information S1): the initially fine powder rings progressively evolve into spotty or single-crystal-like patterns, reflecting grain growth and recrystallization in regions that remain below the local solidus temperature. Therefore, although changes in peak intensities and in texture provide valuable context for assessing near-melt behavior, they reflect micro-structural reorganization during heating rather than the solidus itself. We thus consider these phenomena, but rely on the appearance of liquid diffuse scattering with the pixel-level analysis as the most robust criterion for identifying melting in our XRD experiments.

### 3.4. Comparison With Previous Fe–Ni–Si Studies and Implications

A broader comparison with previous Fe–Ni–Si melting studies conducted using different diagnostics (temperature plateau, diffuse X-ray scattering, ex situ sample characterization) and techniques (XRD, X-ray absorption spectroscopy, shock melting, inter-metallic diffusion in multi-anvil press) highlights the continued development of melting detection approaches (Figure 7). Earlier static compression melting studies employed different combinations of melting proxies. For example, Asanuma et al. (2010) inferred melting from laser power–temperature plateaus together with textural analysis of recovered samples. Morard et al. (2011) and Fischer et al. (2012) identified melting from the appearance of diffuse scattering in XRD patterns, whereas Fischer et al. (2013) combined diffuse scattering with laser power–temperature plateaus. More recently, Edmund et al. (2022) constrained the solidus of Fe–Si alloys using diffuse scattering alone. Beyond static compression experiments using laser-heated DACs, Y. Zhang et al. (2018) constrained the melting of an Fe–Ni–Si alloy using

shock compression, whereas Ezenwa et al. (2024) constrained the solidus of Fe-Si alloys using inter-metallic diffusion in multi-anvil press. These developments reflect both advances in experimental capabilities and the evolving understanding of melting diagnostics. In the present study, the combination of SMS and XRD diagnostics provides two independent and complementary constraints on melting: SMS detects the transition of atomic dynamics through the collapse of hyperfine parameters, while XRD captures the appearance of liquid diffuse scattering.

A key improvement of this study lies in the pixel-level background analysis of diffuse scattering signals in XRD measurements to constrain the solidus of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ . This approach allows for the precise identification of the onset of melting through subtle increases in diffuse intensity, while minimizing contributions from background fluctuations. Although the present method does not allow the liquidus to be quantitatively constrained, it provides a more accurate measurement of the solidus compared to traditional qualitative or integrated-intensity approaches. We also note that the absence of successfully recovered samples suitable for post-mortem compositional analysis currently limits the direct evaluation of possible compositional redistribution during melting. As demonstrated in Figure 2, our refined analysis isolates subtle diffuse signals that were previously indistinguishable from the background, significantly improving the sensitivity and precision of XRD-based melting detection at high pressure and temperature.

As summarized in Figure 7, the reported melting temperature of Fe(-Ni)-Si alloys spans a wide range, even at comparable pressures. Previous studies indicate that Ni has a relatively modest effect on the melting temperature of Fe compared with Si. Static compression experiments on pure Ni (Boccatto et al., 2017; Lord et al., 2014) and Fe-Ni alloys (D. Zhang et al., 2016; Torchio et al., 2020), together with recent shock-compression studies on Ni and Fe-Ni alloys (Pereira et al., 2025; Polsin et al., 2024), generally report melting temperatures comparable to those of pure Fe over similar pressure ranges, despite employing different experimental techniques and melting diagnostics. These observations suggest that the pronounced melting depression observed in the present study is primarily associated with the incorporation of Si. Earlier experiments on Fe(-Ni)-Si with Si contents from 16 to 30 at.% generally cluster near or above the Fe and Fe-Ni solidi, with melting temperatures exceeding 3000 K by 70–80 GPa. More recent studies on Fe-Si systems, including Edmund et al. (2022) and Ezenwa et al. (2024), have also reported substantial solidus temperature depression associated with silicon incorporation. While direct comparison of absolute solidus depression depends on the choice of reference Fe melting curve, these studies collectively indicate that Si can significantly reduce solidus temperatures in Fe-based alloys. Within this broader context, the  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  solidus constrained in this study suggests enhanced melting depression at a Si concentration of 10 at.%.

Extrapolation of the *hcp*- $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  solidus curve to the inner core boundary (ICB) pressure of 329 GPa yields  $4800 \pm 400$  K, which is lower than the melting point of Fe reported by Sinmyo et al. (2019) ( $5500 \pm 220$  K at the ICB pressure). Assuming an adiabatic outer core with a Grüneisen parameter  $\gamma = 1.5$  (Hirose et al., 2013), the corresponding geotherm yields a temperature of  $3520 \pm 290$  K at the core-mantle boundary (CMB) for a  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  core. Because the estimate is derived from the solidus rather than the liquidus, the resulting  $T_{\text{CMB}}$  likely represents a lower bound. As illustrated in Figure S20 in Supporting Information S1, this lower-bound  $T_{\text{CMB}}$  is consistently lower than the melting temperatures of candidate mantle materials, including (Fe,Al)-bridgmanite (Pierru et al., 2022), peridotite (Fiquet et al., 2010), pyrolite (Pierru et al., 2022), chondrite (Andrault et al., 2011), and FeO (Dobrosavljevic et al., 2023), MORB (Pradhan et al., 2015). We note that several of these solidus temperatures differ from the estimated lower-bound  $T_{\text{CMB}}$  by only a few hundred kelvins. If the actual core geotherm closely follows the liquidus of *hcp*- $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$ , the corresponding CMB temperature could be several hundred kelvins higher, reducing or eliminating the temperature difference with these candidate mantle materials. Whether partial melting occurs at the base of the mantle, however, depends on both the thermal state of the core and the composition of the lowermost mantle, and cannot be determined from the present study alone. In addition, the observed defect order-disorder transition in FeO coincides closely with the estimated  $T_{\text{CMB}}$  (Dobrosavljevic et al., 2023), indicating that FeO-rich regions could experience significant changes in physical properties and may contribute to the observed seismic heterogeneity at the CMB (Jackson & Thomas, 2021).

The dual-technique strategy combining SMS and pixel-resolved XRD analysis offers a robust approach to identify melting under extreme conditions. The excellent agreement between the two diagnostics further strengthens the reported solidus in this study, reducing ambiguities that often arise from relying on a single proxy and single technique. Our results directly constrained the solidus of  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  alloy and demonstrate that

silicon substantially depresses the melting temperature relative to Fe and Fe-Ni alloys. The  $\text{Fe}_{0.8}\text{Ni}_{0.1}\text{Si}_{0.1}$  solidus determined here extends existing melting datasets to core pressures (>136 GPa), and provides an enhanced quantitative framework for future XRD melting studies. Together, these advances provide an improved methodological framework for experimental determination of melting under extreme conditions.

## Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

## Availability Statement

All data supporting the findings of this study are available at the Caltech DATA repository <https://doi.org/10.22002/567vt-vmp89> (Zhou et al., 2026). The open-source software MINUTI used for data processing and analysis is available at <https://www.nrixs.com> (Sturhahn, 2025b).

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