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Grüneisen parameter of ε-iron up to 300 GPa from in-situ X-ray study

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ABSTRACT

We show that high-quality powder X-ray diffraction data, collected in diamond anvil cells, provide sufficient information for Rietveld refinement and determination of temperature factors. For the first time using a new method based on combination of thermal equation of state and measured mean-square atomic vibrations of high-pressure ε-Fe phase, we determine Debye temperatures at pressure up to 300 GPa and temperature over 1000 K. We found that the Grüneisen parameter of ε-iron could be described by Anderson's (1967) equation with parameters γ_0 = 1.78(6), q = 0.69(10) with fixed V_0 = 6.73 cm^3/mol.