The goal of your abstract is to convey specific information about your work to your audience

American Mineralogist, Volume 107, pages 248–256, 2022

Ab initio study of structural, elastic and thermodynamic properties of Fe_3S at high pressure: Implications for planetary cores

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ABSTRACT

Using density functional theory electronic structure calculations, the equation of state, thermodynamic and elastic properties, and sound wave velocities of Fe_3S at pressures up to 250 GPa have been determined. Fe_3S is found to be ferromagnetic at ambient conditions but becomes non-magnetic at pressures above 50 GPa. This magnetic transition changes the c/a ratio leading to more isotropic compressibility, and discontinuities in elastic constants and isotropic sound velocities. Thermal expansion, heat capacity, and Grüneisen parameters are calculated at high pressures and elevated temperatures using the quasiharmonic approximation. We estimate Fe-Fe and Fe-S force constants, which vary with Fe environment, as well as the $^{56}Fe/^{54}Fe$ equilibrium reduced partition function in Fe_3S and compare these results with recently reported experimental values. Finally, our calculations under the conditions of the Earth's inner core allow us to estimate a S content of 2.7 wt% S, assuming the only components of the inner core are Fe and Fe_3S, a linear variation of elastic properties between end-members Fe and Fe_3S, and that Fe_3S is kinetically stable. Possible consequences for the core-mantle boundary of Mars are also discussed.

Keywords: Fe_3S, first-principles calculations, high pressure, thermodynamic properties

Things to include in an abstract:

- WHAT you did
- WHY you did it
- HOW you did it
- WHAT you found out
- WHY it is important

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Your introduction is the place to provide background information!

American Mineralogist, Volume 107, pages 262–273, 2022

Improving grain size analysis using computer vision techniques and implications for grain growth kinetics

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Abstract

Earth's physical properties and mantle dynamics are strongly dependent on mantle grain size, shape, and orientation, but these characteristics are poorly constrained. Experimental studies provide an opportunity to simulate the grain growth kinetics of mantle aggregates. The experimentally determined grain sizes can be fit to the normal grain growth law ($G^n - G_0^n$) = $k_0 t \cdot \exp(-\Delta H/RT)$ and then be used to determine grain size throughout the mantle and geological time. The grain growth dynamics of spinel-orthopyroxene mixtures in the upper mantle are modeled here by experimentally producing small grain sizes in the range of 0.5 to 2 μm radius at pressures and temperatures equivalent to the spinel lherzolite stability field. To accurately measure the sizes of these small grains, we have developed a computer vision workflow; using a watershed transformation, which rapidly measures 68% more grains and produces a 20% improvement in the average grain size accuracy and repeatability when compared with manual methods. Using this automated approach, we have been able to identify a significant proportion of small grains, which have been overlooked when using manual methods. This additional population of grains, when fit to the normal grain growth law, highlights the influence of improved accuracy and sample size on the estimation of grain growth kinetic parameters. Our results demonstrate that automatic computer vision enables a systematic, fast, repeatable method of grain size analysis, across large data sets, improving the accuracy of experimentally determined grain growth kinetics.

Keywords: Grain growth kinetics, advanced image processing, watershed algorithm, grain size analyses

Would we be able to find this in a textbook?

Can we quantify this information more effectively?