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D. Daisenberger, M. Wilson, P. F. McMillan, R. Quesada Cabrera, M. C. Wilding, D. Machon, *Physical Review B*, **75**, 224118 (2007)

Abstract:

A low- to high-density pressure-driven phase transition in amorphous silicon is investigated by synchrotron x-ray diffraction in the diamond anvil cell. Complementary atomistic molecular dynamics computer simulations provide insight into the underlying structural transformations and allow us to interpret the structure factors obtained from experiment. During compression the form of the scattering function S(Q) changes abruptly at 13.5 GPa, indicating significant structural rearrangement in the amorphous solid. In particular, the first peak in S(Q) shifts to larger Q values. The changes are correlated with the occurrence of a low- to high-density (LDA-HDA) polyamorphic transition observed previously using Raman scattering and electrical conductivity measurements. The data are analyzed to provide real space (pair distribution function) information. The experimental data are compared with results from molecular dynamics (MD) simulations using a modified Stillinger-Weber many-body potential energy function in order to extract structural information on the densified amorphous material. We deduce that the polyamorphic transition involves an abrupt increase in the proportion of 5- and 6-coordinate Si atoms. The overall structure of the HDA polyamorph can be related to that of the LDA form by creation of highly-coordinated “defects” within the tetrahedrally-bonded LDA network. However, classical and quantum MD simulations indicate that an even higher density amorphous state might exist, based on structures that resemble the densely-packed metallic polymorphs of crystalline Si.