

Abstract Submitted
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Germanene-like defects in Reverse Monte Carlo model of amorphous germanium revealed through new visualization method AL RAHEMTULLA, Univ of Guelph, BRUNO TOMBERLI, Capilano University, EDWARD KIM, University of Guelph, SJOERD ROORDA, Universite de Montreal, STEFAN KYCIA, University of Guelph — High Resolution x-ray diffraction experiments of amorphous germanium (a-Ge) revealed structural differences that cannot be reconciled with accepted theoretical models. An intuitive computational technique has been developed to construct 3D statistical density maps to directly resolve local atomic structure of a-Ge. A reverse monte carlo routine is used to compare the continuous random network model to the experimental model of a-Ge. Undercoordination in the refined model is shown to exist bimodally, as a 4-coordinated tetrahedron and a buckled 3-coordinated structure similar to germanene. These structures account for 95.7% of the total atoms in an approximate 5:2 ratio respectively.

Al Rahemtulla
Univ of Guelph

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