

1096-82-1331

Bridget K Toomey* (toomeybr@math.miami.edu), **Chen Dan Dong**, **Xuchen Han** and **Verne Edward**. *Novel Approach for Evaluating Phases and Orientations of Polycrystalline Structures*. Preliminary report.

Rapid progress in material design has stimulated the need for the development of new tools for efficient and accurate identification of new structure features and properties. This task is relatively straightforward in the case where the new materials are either purely crystalline or purely amorphous. However, these structures are generally new unknown polycrystalline structures that are hard to describe or identify, as they can be made of different regions characterized by different morphology, element types, and orientations. Since the crystal structures and orientations of these composites are vital in understanding and manipulating their properties, researchers require an accurate characterization of the morphological properties at each region. However, no existing software can characterize polycrystals from the positions of their atoms. Therefore, it is urgent to develop such tools. Our method rectifies this gap in crystallography research by designing an algorithm based on the lattice reduction approach (Krivy and Gruber 1976), which has been used in monocrystalline identification. We modify Krivy and Gruber's algorithm to accommodate polycrystalline and amorphous, non-crystalline structures. (Received September 15, 2013)