Materials Science & Engineering Seminar Series

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Simulating Grain Boundaries at the Atomic Scale: More Complicated Than You Think

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ABSTRACT:
The grain microstructure is well-known to have a profound influence on the properties of materials so there is great interest in the properties of grain boundaries. Atomic-scale simulations have been used to study grain boundary properties for over three decades, but there are still many unanswered questions. This reflects the complexity associated with the five geometric degrees of freedom, temperature, and alloy additions and impurities. In this talk, some of the successes and insights from these studies will be highlighted along with some of their pit-falls. These topics range from structure and interfacial defects in pure metals to complexity of alloy segregation.

BIOGRAPHY:
Stephen Foiles is a Distinguished Member of Technical Staff at Sandia National Laboratories in the Computational Materials and Data Science department. He received a BS in Physics from Stanford University in 1978 and a PhD in Theoretical Physics from Cornell University in 1983. His research focuses on the development and application of atomic-scale simulation methodologies, the application of these methods to the study of defects and interfaces, and the connection of these studies with mesoscale materials descriptions. He is a fellow of the Institute of Physics and the American Physical Society.

Doherty Hall 2315, 11:30AM
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