In my last meeting with Professor Fine I entered his office to find him staring at a ball and stick model that he had built of a deformation twin in an hcp structure. He explained to me how he had some ideas about how these defects behaved in Mg alloys based on simple geometrical principles. This talk will highlight very recent work that we have undertaken applying first-principles density-functional-theory calculations in the study of the energetics of deformation twins in hcp transition metals, a class of materials that find widespread use in applications spanning aerospace to nuclear to biomedical devices.

Systematic studies of twin-boundary energetics show clear trends with the filling of the d band, with anomalous behavior discovered near the middle of the transition-metal series. These anomalies correlate with experimental observations on deformed hcp rhenium that are shown to be unusual for hcp metals. We speculate how these findings might impact design of new refractory materials, and show some preliminary results in this direction. Further, we show that the origin of the anomalous behavior stems from the nature of the local atomic geometry in the twin boundary planes. Had we taken the time to visualize the structures in the style of Professor Fine, we could have appreciated the effect much earlier.

Biography:
Professor Asta received his PhD in an interdisciplinary Materials Physics program from the University of California, Berkeley, in 1993. He subsequently joined Sandia National Laboratories at Livermore, CA, as a postdoctoral researcher and then as a senior member of technical staff beginning in 1995. He joined the faculty of the Department of Materials Science and Engineering, Northwestern University, as an Associate Professor in 2000. In 2005 he joined the University of California, Davis, as a full Professor in the Department of Chemical Engineering and Materials Science, where he served as vice-chair from 2008-2009. In 2010 he joined the Department of Materials Science and Engineering (MSE) at the University of California, Berkeley, and the Lawrence Berkeley National Lab. In 2012 he was appointed Department Chair of MSE at Berkeley, and in 2015 he was named the Arthur C. and Phyllis G. Oppenheimer Professor in Advanced Materials Analysis.