Predicting Polymorphic Phase Stability in Multilayered Thin Films

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Abstract

As individual thin film layers in a multilayered stack are reduced in thickness, polymorphic phase transitions can result in which a phase not observed in the standard state is stabilized. These pseudomorphic phases are often serendipitously discovered in the laboratory. A classical thermodynamic model will be presented that can be used in the prediction of polymorphic phase stability in multilayered thin films. An outcome of the model is a new type of phase stability diagram, referred to as the biphase diagram, which can predict pseudomorphic phase stability as a function of length scale and volume fraction. The model has been successfully applied in the prediction and confirmation of hexagonal close packed (hcp) to body centered cubic (bcc) phase stability changes in Zr and Ti for Zr/Nb and Ti/Nb multilayered thin films, respectively. Modeling of the hcp to bcc interfacial energy reduction upon transformation has been coupled to the classical thermodynamic predictions. Additionally, the classical thermodynamic model predicted a novel bcc to hcp Nb phase transformation for each multilayer system. Unlike Zr and Ti that undergo an allotropic phase transformation from hcp to bcc at elevated temperatures, no such equilibrium phase transition is reported for bcc to hcp Nb. X-ray and electron diffraction techniques have been used to identify these changes in phase stability. The compositional structure of the hcp to bcc phase stability in Ti for Ti/Nb will further be addressed in terms of Atom Probe Tomography results.

Dr. Gregory Thompson is currently an assistant professor in the Department of Metallurgical and Materials Engineering at the University of Alabama. Prior to joining the department in August of 2003, Dr. Thompson was a Post-Doctoral Fellow for the Center for the Accelerated Maturation of Materials (CAMM) at The Ohio State University in Columbus, OH. Dr. Thompson's research emphasis is in the processing, phase stability, and functional properties of nanoscaled materials. He received his Ph.D. and M.S. degrees from the Department of Materials Science and Engineering at The Ohio State University in 2003 and 1998 respectively. Previous to his doctoral degree, Dr. Thompson worked as a process engineer for the Southeast Regional Coating Center of Ion Bond, Inc. in Greenville, S.C. He holds a B.S. degree in physics with a minor in mathematics from Brigham Young University in Provo, UT.