Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Prediction of elastic and vibrational stability for Sc, Ti, Y, Zr, Tc, Ru, Hf, Re, and Os in the fcc structure ROMEO DE COSS, EDUARDO CIFUENTES-QUINTAL, Department of Applied Physics, Cinvestav-Merida, Mexico, AARON AGUAYO, GABRIEL MURRIETA, Facultad de Matematicas, Universidad Autonoma de Yucatan, Mexico — The discovery of a metastable phase for a given material is interesting because corresponds to a new bonding and new properties are expected. The calculation of the total-energy along the Bain path is frequently used as a method to find tetragonal metastable states. However, a local minimum in the tetragonal distortion is not a definitive proof of a metastable state, and the elastic and vibrational stability needs to be evaluated. In a previous work, using the elastic stability criteria for a cubic structure, we have shown that the transition metals with hcp ground state; Ti, Zr, and Hf have a fcc metastable phase. That result is interesting since the fcc crystal structure does not appear in the current pressure-temperature phase diagram of these metals, and support the experimental observations of fcc Ti and Zr in thin films. In the present work, we extend the stability study of the fcc structure to the non-magnetic transition metals with hcp ground state; Sc, Ti, Y, Zr, Tc, Ru, Hf, Re, and Os. We find that all the metals involved in this study have a metastable fcc structure, since the phonon band structure shows only positive frequencies. Finally, substrates on which the fcc structure of these metals could be growth epitaxially are predicted.

Romeo de Coss
Department of Applied Physics, Cinvestav-Merida, Mexico

Date submitted: 14 Nov 2013 Electronic form version 1.4