Abstract Submitted for the DAMOP06 Meeting of The American Physical Society

Atomistic Modeling of Segregation and Alloying in Epitaxial Ag films on Al(100) CARY PINT, Dept. of Physics, University of Northern Iowa, USA, GUILLERMO BOZZOLO, NASA Glenn Research Center/Ohio Aerospace Institute, USA, RICHARD SMITH, Dept. of Physics, Montana State University, USA, JORGE GARCES, Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Argentina — The Bozzolo-Ferrante-Smith (BFS) method for alloys is applied to the study of interfacial alloying and interdiffusion in epitaxial Ag layers on Al(100). For submonolayer coverage, Ag is seen to first grow epitaxially until bulk diffusion sets in at higher temperatures. The presence and magnitude of this diffusion energy barrier has significant consequences for Ag films on Al(100), where stable layers of Ag are formed on the Al(100) substrate at low temperatures. This is followed by a progressive segregation of the Ag atoms into the Al bulk upon heating, accompanied by the formation of a stable interfacial compound. This behavior becomes more pronounced with higher Ag coverage. A simple analysis of the energetics indicates interesting trends during this process- particularly a chemical energy transition that shifts to higher temperatures with increasing Ag coverage. The results from this simple modeling technique seem to be in agreement with the behavior of Ag/Al(100) established through previous experiment.

Cary Pint Dept. of Physics, University of Northern Iowa, USA

Date submitted: 26 Jan 2006

Electronic form version 1.4