2003 TMS 132 Annual Meeting and Exhibition: The TMS 2003 International Metals and Materials Exhibition, San Diego, California, March 2–6, 2003

(Invited)

BISMUTH INDUCED EMBRITTLEMENT OF COPPER GRAIN BOUNDARIES

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Catastrophic brittle fracture of crystalline materials is one of the best documented but least understood fundamental phenomena in materials science. A common feature of most materials that exhibit brittle fracture is the segregation of impurity elements to grain boundaries. Embrittlement of copper by bismuth is the classic example of this phenomenon. In this study, we use a combination of atomic resolution Z-contrast imaging, electron energy-loss spectroscopy and density functional theory to investigate the geometric and electronic structure of a copper grain boundary with and without bismuth. We are able to resolve the atomic arrangement of the bismuth doped boundary, detect impurity-induced changes in the electronic structure and calculate the charge density in the vicinity of Bi impurities. These results suggest that the copper atoms that bond to the segregated bismuth become embrittled by taking on a zinc-like electronic structure.