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Continuum Description of Atomistics for Nanomechanics of Grain Boundary Embrittlement in FCC Metals K.-S. KIM, C.-K. WANG, M.-H. CHA, H. B. CHEW, School of Engineering, Brown University — A nonlinear field projection method has been developed to study nanometer scale mechanical properties of grain boundaries in nanocrystalline FCC metals [1]. The nonlinear field projection is based on the principle of virtual work, for virtual variations of atomic positions in equilibrium through nonlocal interatomic interactions such as EAM potential interaction, to get field-projected subatomic-resolution traction distributions on various grain boundaries. The analyses show that the field projected traction produces periodic concentrated compression sites on the grain boundary, which act as crack trapping or dislocation nucleation sites. The field projection was also used to assess the nanometer scale failure processes of Cu $\Sigma 5$ and $\Sigma 9$ grain boundaries doped with Pb. It was revealed that the most significant atomic rearrangement is dislocation emission which requires local GB slip, and some Pb locks the local GB slip and in turn, embrittles the GB. Reference: [1] C.-K. Wang, et al., 2011, *MRS Proceedings*, Vol. 1297, DOI: 10.1557/opl.2011.678.

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