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Modified Young's equation for equilibrium dihedral angles of grain boundary grooves in thin films at the nanoscale MING-WEI LIU, SHANG-CHUN LIN, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, MOGADALAI GURURAJAN, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology-Bombay, Powai Mumbai, India, KUO-AN WU, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — We derive the modified Young's equation for the equilibrium dihedral angle at the triple junction of the grain boundary groove by taking into account the discrete structure of the low angle grain boundary. For low angle grain boundaries, the geometric relation that the misorientation of the bicrystal is inversely proportional to the dislocation spacing naturally gives rise to the variation in the misorientation when the grain boundary length changes (holding the number of dislocations constant). The fact that the grain boundary energy increases as the grain boundary length decreases due to a smaller dislocation spacing leads to a larger dihedral angle compared to that of the classical theory. Two atomistic continuum modelling tools, namely the phase field crystal model and the amplitude equations, are used to simulate the equilibrium dihedral angle. The numerical results are in quantitatively good agreement with the derived modified Young's equation.

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