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The Structure of (001) CSL Twist Boundaries in fcc Metals

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Abstract: Computer simulation techniques based on discrete lattice approach and empirical many-body potentials have been used to study the structure and energy of $\Sigma = 5$, and $\Sigma = 13$ coincident site lattice (001) twist boundaries in three fcc metals. Energy computed for $\Sigma = 5$ boundary in copper is 17.5 % less than the earlier result obtained by using pair potential. However the present calculations of twist boundary energies are somewhat higher than the results obtained using embedded atom method.

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