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Multiple Structures of (110) CSL Twist Boundaries in fcc Metals

Abdul GHAFOR, Barkat Ali Shafiq FARIDI, Aftab AHMAD
Department of Physic, Islamia University,
Bahawalpur-PAKISTAN

Abstract: The geometry of different possible structures of (110) fcc twist boundaries is explored. Computer simulation of all possible low energy structures have been carried out for $\Sigma=3$ and $\Sigma=9$ twist boundaries using many-body potentials representing copper, silver and gold. Low symmetry structures are found to have lower energies than the high symmetry CSL structures.

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