

Maximum or minimum Density Principle determines the bulk Terminations of Quasicrystals?

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In [1] we announced the “thick layer” concept of the bulk terminations in quasicrystals. We consider a bundle of dense atomic planes in the bulk, not necessarily extremely close together, as a candidate for a termination. We show that only “thick” layers can terminate the bulk of decagonal Al-Cu-Co (d-AlCuCo) in the 2fold directions. Also, the secondary electron images indicate that certain “thick” 5fold and 2fold layers are favoured as terminations of icosahedral Al-Pd-Mn (i-AlPdMn). In particular, the 2fold terrace-like surfaces of i-AlPdMn containing pits are perfectly explained in this framework.

Following a suggestion of Sharma et al. [2], that a gap in the bulk might define a termination, we introduce a minimum density rule on low density “thick” atomic layers as well and show that, in the framework of the model of i-AlPdMn, such a rule does not match the observed step heights on either the 2fold or 5fold surfaces.

[1] Papadopolos Z. et al., *Phys. Rev. B*, 2004, **69**, 224201. [2] Sharma H.R. et al., *Phys. Rev. Lett.*, 2004, **93**, 165502.

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