Wulff shape emergence and sharp $n^{3/4}$ law for crystals

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In this talk the problem of understanding why particles self-assemble in macroscopic clusters with overall polyhedral shape is investigated. At low temperature ground states for a general finite number n of particles of suitable phenomenological energies possibly accounting for two- and three-body atomic interactions are shown to be connected subsets of regular lattices $\mathcal{L}$, such as the triangular and the hexagonal lattice. By means of a characterization of minimal configurations via a discrete isoperimetric inequality, ground states will be seen to converge to the hexagonal Wulff shape as the number n of particles tends to infinity. Furthermore, ground states are shown to be given by hexagonal configurations with some extra particles at their boundary, and the $n^{3/4}$ scaling law for the deviation of ground states from their corresponding hexagonal configurations is shown to hold. Precisely, the number of extra particles is carefully estimated to be at most $K_{\mathcal{L}}\, n^{3/4} + \mathrm{o}(n^{3/4})$, where both the rate $n^{3/4}$ and the explicitly determined constant $K_{\mathcal{L}}$ are proven to be sharp. The new designed method allows to sharpen previous results [1, 5] for the triangular setting [2] and allows to provide a first analytical evidence of the zigzag-edge selectivity and the emergence of the asymptotic Wulff shape for the hexagonal setting [3] in accordance with what is experimentally observed in the growth of graphene flakes [4]. Results presented are in collaboration with Elisa Davoli and Ulisse Stefanelli (Vienna).

References

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