

Dislocation problems for periodic Schrödinger operators and mathematical aspects of small angle grain boundaries

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In many mathematical models for periodic crystals, the crystal atoms are assumed to be on the lattice sites of a periodic lattice Γ , under the influence of a Γ -periodic potential V , so that the energy levels of the crystal are described by the spectrum of the Schrödinger operator $-\Delta + V$. However, in real crystals, the regular periodic pattern of atomic arrangement is interrupted by crystallographic defects. In this talk, we study models for a translational defect as well as a small angle defect in two-dimensional lattices. We begin with dislocation problems in one dimension and on the strip $\mathbb{R} \times (0, 1)$ to motivate our technical tools and to establish some basic results. Our first goal is to compute estimates for the density of surface states in dislocation problems on \mathbb{R}^2 . Secondly, for a small angle grain boundary with angle $\vartheta > 0$, we show that the spectral gaps of the periodic problem fill with spectrum as $\vartheta \downarrow 0$. The talk is based on a joint work with R. Hempel.