Flat Energy Bands within Antiphase and Twin Boundaries and at Open Edge in Topological Materials

SUPPLEMENTAL MATERIAL

Linghua Zhu,1 Emil Prodan,2 and Keun Hyuk Ahn1

1Department of Physics, New Jersey Institute of Technology, Newark, New Jersey 07102, USA
2Department of Physics, Yeshiva University, New York, New York 10016, USA

LATTICE ENERGY FOR RELAXED STRUCTURAL TEXTURES

Lattice distortion field should satisfy the compatibility conditions, that is, the bonds between atoms should not be broken or overlap with each other. Further, abrupt changes in lattice distortions usually cost a lot of lattice energy, and gradual changes of the lattice distortions would be favored energetically. To take both effects into account at the atomic scale, structural textures are obtained by relaxing an energy expression \(E_{lattice}\) written in terms of the atomic scale modes that represent the lattice distortions. Specifically, the distortion of a square lattice with a monatomic basis can be expressed in terms of five distortion modes, \(e_1, e_2, e_3, s_x,\) and \(s_y,\) shown in Fig. S1, as discussed in detail in Refs. [S1–S4]. The energy expression \(E_{lattice}\), which gives rise to the ground states with \(e > 0, d_x = 0, d_y \neq 0\) (equivalently with \(e < 0, d_x \neq 0, d_y = 0\)) illustrated in Fig. 1 is as follow

\[
E_{lattice} = E_s + E_l + E_c, \tag{S1}
\]

\[
E_s = \sum_i \left[ \frac{B}{2} (s_x^2 + s_y^2) + \frac{G_1}{4} (s_x^4 + s_y^4) + \frac{G_2}{2} s_x^2 s_y^2 \right], \tag{S2}
\]

\[
E_l = \sum_i \left[ \frac{A_1}{2} e_1^2 + \frac{A_2}{2} e_2^2 + \frac{A_3}{2} e_3^2 \right], \tag{S3}
\]

\[
E_c = \sum_i \left[ C_3 (s_x^2 - s_y^2) e_3 \right]. \tag{S4}
\]

where \(E_s\) is the energy for the short-wavelength modes including all symmertry-allowed terms up to the fourth order, \(E_l\) the energy for the long-wavelength modes in the harmonic order, \(E_c\) the coupling between the long- and short-wavelength modes, and \(i = [i_x, i_y]\) designates coordinates before distortion.

For uniform phase, the energy minimization of \(E_{lattice}\) leads to \(e_1 = e_2 = 0\) and \(e_3 = -C_3 (s_x^2 - s_y^2)/A_3\), and the minimized total energy per site is

\[
\frac{E_{tot,min}}{N^2} = \frac{B}{2} (s_x^2 + s_y^2) + \frac{1}{4} \left( \frac{G_1}{A_1} - \frac{2C_3^2}{A_3} \right) (s_x^4 + s_y^4) + \frac{1}{2} \left( \frac{G_2 + 2C_3^2}{A_3} \right) s_x^2 s_y^2. \tag{S5}
\]

With \(B < 0, G_1 - 2C_3^2/A_3 > 0, G_2 + 2C_3^2/A_3 > 0,\) and \(G_2 + 2C_3^2/A_3 > G_1 - 2C_3^2/A_3,\) the global energy minimum occurs for \(s_x = \pm s_{min}, s_y = 0\) and equivalently for \(s_x = 0, s_y = \pm s_{min},\) where \(s_{min} = \sqrt{BA_1}/(2C_3^2 - G_1 A_3).\) For the results in the main text, the parameter values are chosen as \(A_1 = 7, A_2 = 4, A_3 = 6, B = -5, C_3 = 20, G_1 = 180,\) and \(G_2 = 100,\) which satisfy the conditions specified above and give the minimum energy distortion \(s_{min} = 0.327\) and \(e_3^{min} = 0.357,\) equivalently \(e = 0.252\) and \(d_x = 0.164, d_y = 0\) or \(d_x = 0, d_y = 0.164\) in Fig. 1. For the inhomogenous configurations with TB and APB, the constraints among \(e_1(k), e_2(k), e_3(k), s_x(k),\) and \(s_y(k)\) should be considered.

![FIG. S1: Atomic scale distortion modes for a square lattice [S1–S4]. The modes \(e_1, e_2\) and \(e_3\) are long wavelength modes, and the modes \(s_x\) and \(s_y\) are short wavelength modes.](image-url)
as done in Refs. [S1–S4]. With appropriately chosen initial configurations, the lattice configuration is relaxed using the Euler method applied to $E_{\text{lattice}}$ to obtain the atomic scale profiles of TB, APB, and the zig-zag boundaries in Figs. 2-4 of the main text.