Ab initio study of anisotropic mechanical properties of $LiCoO_2$ during lithium intercalation and deintercalation process

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The mechanical properties of Li_xCoO_2 under various Li concentrations and associated anisotropy have been systematically studied using the first principles method. During the lithium intercalation process, the Young's modulus, bulk modulus, shear modulus, and ultimate strength increase with increasing lithium concentration. Strong anisotropy of mechanical properties between a-axis and c-axis in Li_xCoO_2 is identified at low lithium concentrations, and the anisotropy decreases with increasing lithium concentration. The observed lithium concentration dependence and anisotropy are explained by analyzing the charge transfer using Bader charge analysis, bond order analysis, and bond strength by investigating partial density of states and charge density difference. With the decrease of Li concentration, the charge depletion in the bonding regions increases, indicating a weaker Co-O bond strength. Additionally, the Young's modulus, bulk modulus, shear modulus, and toughness are obtained by simulating ab initio tensile tests. From the simulated stress-strain curves, Li_xCoO_2 shows the highest toughness, which is in contraction with Pugh criterion prediction based on elastic properties only.