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Outline of Thesis

Title: Theoretical Analysis of Deformation Mechanisms in Graphite Layered Composites

This thesis is composed of five chapters, the composition of the entire thesis is as follows.

Chapter 1 "General Introduction" introduced the research background and objectives of this thesis. It provided a detailed overview of the current state of research on layered solid materials, the deformation mechanisms of layered structural materials, and the mechanical models of layered structural materials.

Chapter 2 "Molecular Dynamics Studies on Mechanical Properties and Deformation Mechanism of Graphene/Aluminum Composites" investigates the mechanical properties of graphene/aluminum (Gr/Al) composite materials under uniaxial tension and compression using molecular dynamics (MD) simulations. This chapter demonstrates that graphene serves as an excellent reinforcement material, significantly enhancing the Young's modulus when combined with pure aluminum. Additionally, a phase transition structure during compression is analyzed using radial distribution function (RDF). Furthermore, this chapter includes the measurement of the mean curvature and Gaussian curvature of the compressed graphene surface and takes into account the deformation characteristics of graphene within the composite using the differential geometric method. A novel approach based on atomic coordinates is applied to calculate surface curvature and material deformation, introducing a new perspective for assessing material deformation in three-dimensional space. And in the compressive deformation of van der Waals crystalline materials, plastic deformation is based on the nucleation and propagation of ripplocation and not on basal dislocations.

In the chapter 3 "Characterizing the Deformation Mechanism of Ripplocation in Silicon–Graphite Composites", we thoroughly investigated the effects of the number of graphene layers and dimensions on the variation of ripplocations and ripplocation boundaries (RBs) in sandwich-structured graphite–silica composites under lateral loading using molecular dynamics. Further, we derived the bending energy of singlelayer graphene by applying the Helfrich–Hamiltonian theory. Specifically, to study multilayer graphene under specific conditions, which can be analogous to sinusoidal corrugated plates, we developed an effective combination of microscopic simulations and macroscopic theory. We found that the larger the number of layers of graphene and the larger the width, the smaller the number of RBs and the easier it is for RBs of the same sign to attract each other.

In the Chapter 4 “Deformation Mechanism and Minimum Energy Path in Silicon–Graphite Composites with Lattice Defects”, this chapter utilized dynamic simulations to investigate the impact of different types, quantities, and angles of lattice defects on the deformation mechanism of defective graphite. Compared to previous studies, we have included the influence of different lattice defect types in graphene on ripplocation. Additionally, we have utilized the Nudged elastic band method (NEB) method to calculate the minimum formation pathway for these defects.

In the Chapter 5 "General Conclusion", this chapter provides a comprehensive review of the research conducted, offering insights into the findings and outlining prospects for future research endeavors. Specifically, this thesis offers valuable insights into the mechanical behavior of layered solid materials through the lens of molecular dynamics simulations. However, to further enrich the comprehensiveness and applicability of our findings, future research should strive to combine experimental validation with a broader exploration encompassing diverse material types and defect categories.