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**First-principles simulations on chemical transformation bonding pathways of compressed graphite** ANGUANG HU, FAN ZHANG, Defense R&D Canada-Suffield, Canada, Box 4000, Stn. Main Medicine Hat, Alberta, T1A 8K6 Canada — Chemical transformation bonding pathways for cubic diamond, hexagonal diamond, and cold compressed carbon has been investigated using first-principles simulations of the enthalpy minimization with various target pressures. The high-pressure bonding pathways of carbon from initial bonding conformations can be divided into three bonding evolution stages, which are defined as the van der Waals bonding destruction, bond breaking and forming reaction, and bonding equilibrium process. The principal stress tensor components were used to characterize the response of C-C bonds in graphite to compressive loading. It was found that the local stress field starts to rapidly increase towards the positive direction at the onset of the van der Waals bonding destruction. Bond breaking and forming reaction then takes place, leading to a cell volume collapse accompanied with a drop in stress components. The three bonding evolution stages demonstrated that the bonding evolution of the system towards chemical transformation under compression can be dictated by the local stress field together with the initial bonding conformation. Thus, the local stress field provides an understanding on how atoms and electrons move during the course of chemical transformation under compression.

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