Strength and Thermal Stability Characteristics of Graphene-Reinforced Layered Composites Based on Pure Ru And Alloy Ru-Pd

Kurbanova E.D., Polukhin V.A.

Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Yekaterinburg

This paper summarizes the results of MD modeling of thermoactivated relaxation and formation of the metal/graphene interface structures (Me: Pd, Ru/G), their disorder and destruction (analogous to melting in low-dimensional systems) under further heating. The potential functions describing the interactions of the Ru-Ru and Ru-Pd atoms (for the initial palladium-doped Ru/G interface) as well as the interactions of the Ru, Pd atoms with the graphene substrate carbon have been estimated and parameterized using the Sutton-Chen quantum-mechanical immersed atom (EAM) method.
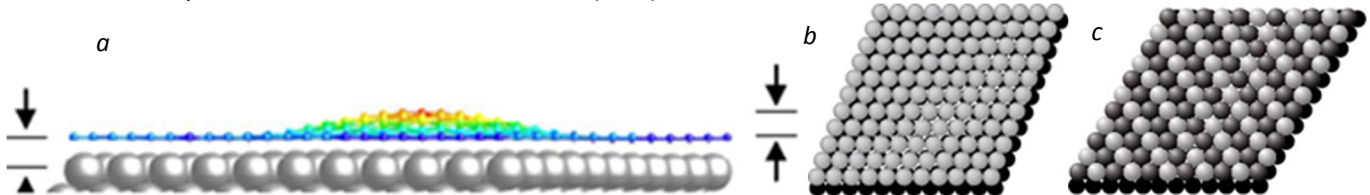

Fig. 1 Coordination configurations of the cell (3.0 nm) of the periodic translation of superstructure I, which was formed during MD simulation of the interface formed during the superposition of the graphene monosheet surface and the (0001) surface of a Ru film: (a) side view, the arrows illustrate the graphene monosheet corrugation amplitude (0.167 nm, right-hand arrows) and distance d between the graphene and Ru planes (0.222, left-hand arrows); (b) top view, 3.0-nm unit cell with 11 × 11 Ru atoms (gray, top plane) and 12 × 12 C atoms (black circles, bottom plane); and (c) 3.0-nm unit cell with 50% substitution of Pd atoms for Ru sites in an Ru film (open circles) with the damping effect of corrugation amplitudes (waviness). The atomic radii are R_{Ru} = 0.134 nm and R_{Pd} = 0.137 nm
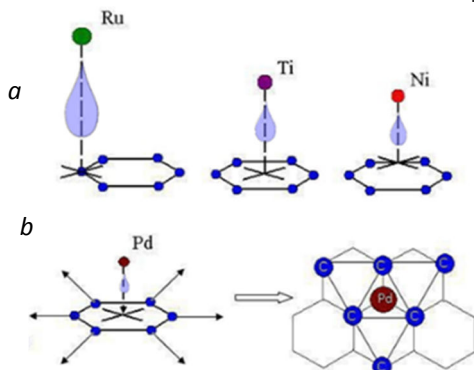

Fig. 2 Electron density distribution in the G/M interface surface as a function of an element and the direction of M–G bonds: (a) side view for Ru, Ti, and Ni atoms over hexagonal graphene; (b) formation of a coordination corner of carbon atoms around a Pd atom in the G/Pd_xRu_{1-x} interface (top view). The crosses indicate the maximum electron density concentration with the formation of a π_z–d_z bond

In contrast to the carbide-forming Ru film and Ru-Pd alloy (like Ti), the Ru and Ru-Pd-based interface is formed by physical adsorption and van der Waals forces, where the Pd atoms are arranged over the hexagonal C atoms of graphene with minimal distortion of Pd-Pd bonds, rather than by chemisorption (π-d hybridization). Moreover, the sorption energy in the chemisorption interfaces is determined by the bonding directions at the C-C bond centre in the Ni/G with contrast interface, at the hexagonal centres in Ru/G, and toward the C atoms in Ru/G).
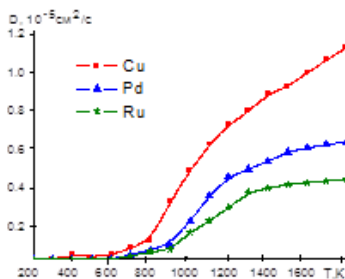

Fig. 3 Temperature dependences of the diffusion coefficients of the metals in M/G (M = Cu, Pd, Ru) interfaces.
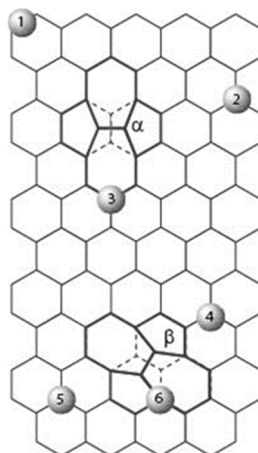

Fig. 4 Fragment of the (12 × 12) graphene plane structure of the unit cell (3.0 nm) of the G/Ru–Pd interface after hydrogenation (see Fig. 1). Numerals indicate hydrogen atoms randomly adsorbed on the graphene plane. Hydrogen atoms at sites 3 and 6 passivate Stone–Wales defects of different types, which have different angles of C–C bond rotation(α = π/2, β = π/4)

It is also shown that the strength characteristics and thermal stability of interfaces with graphene-reinforced metallic films can be improved by the formation of both hydrogenated mutually bonded point defects (Stone-Wales vacancies) and metallic complexes of intercalated dopant atoms, which compensate for strain stresses in parametrically incommensurable configurations of dissimilar atoms.