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Influence of Metal Substrates on the Nucleation of Chemical Vapor Deposition Growth of Graphene¹ JIA LI, LIXIANG ZHONG, Graduate School at Shenzhen, Tsinghua University, Shenzhen 518055, People's Republic of China, YUANCHANG LI, National Center for Nanoscience and Technology, Beijing 100190, People's Republic of China — Using *ab initio* calculations, we systematically investigate the graphene nucleation on ten kinds of metal substrates that have been reported for the chemical vapor deposition growth of graphene. Noble metals (Cu, Ag and Au) and Co have a kinetic smallest graphene precursor, corresponding to the structural transition from linear chain to sp^2 compact cluster. Ru, Rh, Ir and Pt have a energetic smallest graphene precursor, which is much larger than that in terms of kinetics. While for Ni and Pd, the carbon atoms trend to immerse inside the metals, resulting in the distinctively different growth mechanism from other metals. The different influence of metals is associated with their characterized carbon-metal and carbon-carbon coupling competition. The incorporation of five-membered rings into the sp^2 compact cluster is the result of the competition between the curvature energy and the edge formation energy of graphene islands, and is suitable for the enlargement of graphene domain. And the effect of experimental conditions such as temperature, step or defects on the nucleation of graphene at different metal substrates is also discussed.

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