LOW AND HIGH INDEX SURFACES FOR GRAPHENE SYNTHESIS

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Low-index surfaces are commonly preferred in graphene synthesis due to their inherently low surface energy values [1]. Nevertheless, in recent times, there has been an increasing interest in high-index surfaces, which are considered to be better in terms of catalytic activity than low-index surfaces [2]. For this purpose, the surface energies of high-index (310), (311), (331) and low-index (100), (110), (111) nickel surfaces were calculated using molecular dynamics simulations. The results indicate that among the high-index surfaces, the Ni(331) surface exhibited the lowest value of 2.05 J/m², which is 0.01 J/m² less than the surface energy of the Ni(110) surface, which measured 2.06 J/m². These results suggest that high-index Ni(331) surface can be used in graphene synthesis as well as low-index surfaces.



Fig.1 Surface energy values of high and low index nickel surfaces.

REFERENCES

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