Defects and grain boundaries (GBs) greatly influence the properties of graphene but modeling their formation is challenging due to the multiple length and time scales involved.

Phase Field Crystal (PFC) is a continuum approach where the free energy functional describing the system has periodic ground states. It tracks systems on diffusive time scales but retains atomic resolution. Large system sizes can be tackled using the PFC model. [1]

We have applied PFC models to study graphene GB structures and their energy as a function of the tilt angle. Our goal is to gain a better understanding of graphene microstructure which may lead to improvements in processing and new applications.

The GB energy given by the amplitude model agrees with the one-mode model but retains atomic resolution. Large system sizes can be tackled using the PFC model. [1]

The three-mode model produces a rich variety of GB structures most of which have been treated in other works also [4]. The common 5/7 dislocation proved prevalent. The GB energy is in a fair quantitative agreement with other numerical works, Fig. 3 [5].

The one-mode model has a strong preference towards 5/7 dislocations while most other dislocation structures prove unstable. The GB energy is in a qualitative agreement with other numerical works.

The GB energy given by the amplitude model agrees with the one-mode model but saturates at large tilt angles.

CONCLUSIONS

We seek minimum energy GB structures to get a consistent lower limit estimate of the GB energy. Various dislocation types have been identified and their occurrence and energies compared with literature. We have validated the system sizes used with a finite-size effect analysis.

REFERENCES


