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Machine Learning prediction of the structural/textural-mechanical properties relationship of pyrolytic carbons

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The ability of C/C composites to maintain high mechanical properties up to very high temperatures (above 3000 K), combined with their low densities, justifies their use in extreme conditions, especially in aerospace and defense applications. However, due to the very large anisotropy of their constituents, their partial crystalline order, and the difficulty to perform experiments under the appropriate conditions, the relationship between the structure/texture of these materials and their mechanical behavior is incomplete. In particular, the prediction of the individual behavior of the different constituents (fibers, matrices) at small scales is a fundamental step in the development of virtual materials at the composite or part scales.

We propose an original approach to develop atomistic models of Pyrocarbon (PyC) matrices using a molecular dynamics reconstruction method guided by a polygranular textured image (PG-IGAR), introduces explicitly grains (crystallites) in the 3D image template of size (Lc , La) and orientation OA derived from X-Ray diffraction and Selected Area Electron Diffraction data (SAED), respectively. This method is used to provide a large database of relevant structural and textural properties of these materials [1].

The full elastic tensors of the models constituting the database are computed within the adiabatic framework. Doing so, the adiabatic elastic constants are obtained by imposing an instantaneous deformation of the material neglecting both lattice and atomic relaxations. This method has already been used to computed the elastic tensor of the triclinic compound TATB [2] and for single crystalline graphite [3]. Such elastic constants are directly comparable to the measurement of mechanical properties by ultrasonic pulse experiments.

Finally, a Machine Learning (ML) model using random regression tree forests is implemented in order to accurately describe the relationship existing between structure and texture on one side and the mechanical behavior on the other side.

References

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