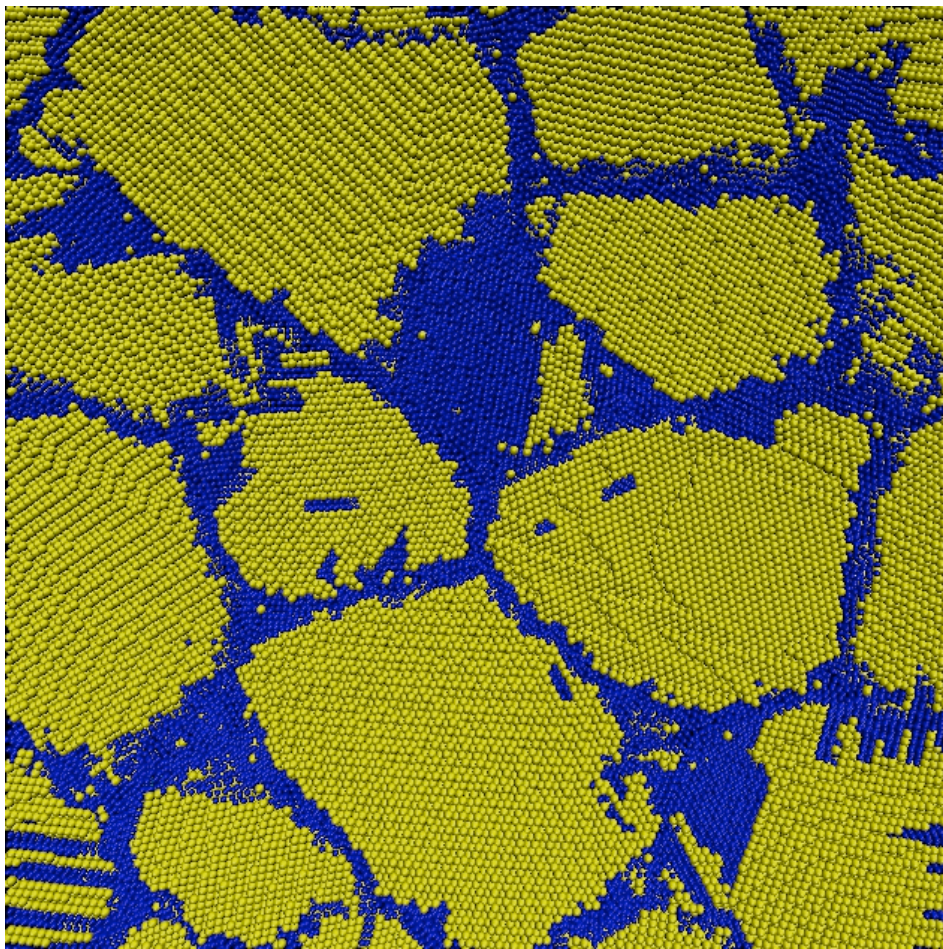


Atomistic study of the mechanical properties of iron and carbon steel

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Iron is one of the most important components of the universe, and is ubiquitous in the Earth crust and Earth interior. It has clear technological relevance, from the 'iron age' till our days, where steels are the structural material of choice in a large variety of settings. In this study I calculate first the elastic properties of Fe-C single crystals and compare them to available experimental data. Secondly, to build a bridge to the dynamical properties of iron and steels I analyze the behaviour of nanocrystalline Fe under extreme pressure conditions by molecular dynamics simulations.

