Atomistic modeling of metallic glasses from first-principles dynamics

Metallic glasses (MG) are amorphous metallic alloys, which are produced by rapid quenching from a molten state at a sufficiently first cooling rate so that crystal nucleation and growth can be avoided. The bulk counterpart of MGs, known as BMGs, possess unique properties, such as higher strength, lower Young's modulus, improved wear resistance and good fatigue endurance, due to the combination of metallic bonding and amorphous structure. Computational studies of MGs/BMGs are primarily related to classical simulations, due to the large size of the models that is necessary to address bulk properties of these glasses.

In our work, we address the structural, electronic, and vibrational properties of $Ni_{40}Pd_{40}P_{20}$ bulk metallic glass using ab initio molecular-dynamics simulations based on density-functional theory by employing a bigger system size and relatively higher cooling rates. Thus far, only a few *ab initio* studies on the electronic and structural properties of $Ni_{40}Pd_{40}P_{20}$ have been reported in literature. The scope of the our *ab initio* study goes much further by addressing the vibrational properties of glassy $Ni_{40}Pd_{40}P_{20}$, starting with a notably larger model and a relatively slower cooling rate than the ones that were used in earlier studies.