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Contributions of atomistic simulations to the understanding of the formation and evolution of defects in crystalline materials

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To tackle the scientific and industrial challenges ahead, the availability of novel high-performance materials will be of prime importance. To this aim, modern laboratories and industries heavily rely on models and numerical simulations to foster the design of tailored properties materials. In this context, atomistic modelling provides a unique access to fundamental material mechanisms able to support innovative physics-based constitutive models for material design.

Here we present the contribution of atomistic simulations towards the development of higher-scale models, though the understanding of the plastic deformation of crystalline materials. The Molecular Dynamics method will be presented and compared with other approaches, such as Density Functional Theory approaches and Monte Carlo simulations. Then, examples of investigations will be presented and discussed. The dislocation absorption in GBs and the influence of internal strain on irradiation-induced damage will be shown as examples of inputs in higher scale models¹. The interplay of atomistic simulations and experiments will be highlighted through the investigation of irradiation damage², the formation of defects in MAX phases^{3,4}, the initiation of plasticity in nanowires^{5,6}, and the dislocation-interface interactions in metallic composites^{7,8} and superalloys⁹. The focus of this lecture will be the inputs provided by these atomistic simulations to higher scale techniques and the interplay with experiments.

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