Seminarium Departamentu Fizyki Materiałów

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On the classification and quantification of material defects in damaged crystalline solids by machine learned based MD simulations and a novel fingerprinting and visualization tool

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In this talk, I will discuss the analysis of damaged crystalline materials by presenting the computation of machine learning (ML) molecular dynamics (MD) interatomic potentials into the Gaussian Approximation Potential framework, to model efficiently the mechanism of energetic particle irradiation on crystalline solids. The obtained simulated damaged materials are then studied by a fingerprint-like method which is based on the calculation of a descriptor vector for each atom in the sample. This method has also been proposed to provide a probabilistic interpretation of identified point defects, e.g. self-interstitial-atoms and vacancies, requiring modest computational resources.

As an application, I will show results of the study of damage in pure and hydrogenated tungsten samples due to neutron bombardment. Common point defects like self-interstitial-atoms and W atom next to a vacancy, as well as vacancies formation, are quantified and classified dynamically at different impact energies. The arrangement of complex defects like dumbbells and crowdions are identified in the sample by our method with a principal component analysis.