# ТЕЗИСЫ ДОКЛАДОВ

## МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ

**«Физическая мезомеханика.
Материалы с многоуровневой иерархически организованной структурой и интеллектуальные производственные технологии»,**

посвященная 90-летию со дня рождения
основателя и первого директора ИФПМ СО РАН
**академика Виктора Евгеньевича Панина**

**в рамках**
**Международного междисциплинарного симпозиума**
**«Иерархические материалы: разработка и приложения для новых технологий и надежных конструкций»**

**5–9 октября 2020 года**
**Томск, Россия**

Томск
Издательство ТГУ
2020

**DOI: 10.17223/9785946219242/102**

## INFLUENCE OF GRAIN STRUCTURE ON THE MECHANISMS OF PLASTICITY NUCLEATION IN BCC METAL UNDER MECHANICAL LOADING

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The study of atomic mechanisms of plasticity nucleation in metallic materials is crucial for design of new materials for different practical applications. Experimental, theoretical and computer simulation studies show that the nucleation of plasticity is realized by structural transformations on the atomic scale [1-5]. The features of these transformations largely depend on the stress distribution which is determined by the internal structure of the material. In view of the small spatial and temporal scales of processes at the microscopic level, computer simulation is one of the most effective approaches for studying the dynamics of plasticity nucleation in materials. In the present work, the influence of the grain structure characteristics and features of stress distribution on the activation of various deformation mechanisms of bcc iron was studied in the framework of molecular dynamics simulation. The nucleation of plasticity under constrained shear deformation in the nanocrystalline iron samples with different grain sizes is investigated. The relationship between the characteristics of the stress distribution in the simulated samples and the strain values at which structural defects are nucleated is established.

*The work was performed according to the Government research assignment for ISPMS SB RAS, project No. III.23.1.4, and Russian Foundation for Basic Research grant No. 16-08-00120.*

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