Molecular Dynamics Modeling of Thermal-induced Structure Reorganization and Residual Stresses Accumulation in Solids

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High temperature exposure of solids induces irreversible changes of the material internal structure. In welded seams such processes lead to accumulation of internal stresses, which can drastically worsen the strength characteristics of the materials and structures. Description of such processes in the frames of the continuum mechanics meets serious problems, since in this case the assumption of the deformation continuity fails, which is the basic assumption for the macroscopic mechanics. The defects of the material internal structure break the internal geometry of the solid resulting in a serious challenge for the strain determination. The realistic theory for media with detect structures can be constructed on the base of non-Euclidean geometrical description of deformations of elastic media. However, in the frames of continuum mechanics it is impossible to answer the questions about the defects initiation mechanism and influence of the thermal processing on the material properties.

In the presented lecture the essentially discrete approach is used for description of the changes in the material internal structure and the residual stresses initiation under the strong thermal action. The method of material modeling using particles is based on the material representation by a set of interacting particles, described by Newtonian equations of motion. The materials properties are determined by the interparticle potential and the initial particle packing. The best developed variant of this method is molecular dynamics method, which is for several decades widely used for description of physical and chemical properties of solids. In general, the representative particles are not necessary associated with atoms and molecules, but can be interpreted as discrete representatives of the material properties. However, in this case also the term “molecular dynamics” is used, but the better choice can be the term “mesoparticle dynamics”. Let us note, that the considered method is discrete on the physical level, which differs it from the other methods with similar names (e.g. smooth particle hydrodynamics, method of big particles and etc.) where the particles are used only as a movable mesh for integrating the continual equations.

In the presented work it is shown how molecular dynamics allows to describe the initiation of the defect structures and residual stresses in the material subjected to strong thermal processing. The sample problem of the non-uniform heating with sequential cooling of the rectangular specimen is considered. The simulation results show that differences in the thermal processing methods can result in different internal structure of the material, in particular the size of the single-crystalline grains can be varied from the real polycrystal to nearly amorphous material. The distribution of the residual stresses produced by the thermal action is considered. Influence of the different types of defects on the stress state in the material is investigated.

The results of the presented investigations prove that in the future the considered method can be successfully used for selecting the optimal regimes for the thermal processing of materials. Until now the molecular dynamics has limited applications in mechanics if solids due to high requirements for the computational power. For example, a cube with an edge of 100 particles contains one million particles, cube with an edge of 1000 particles contains one billion particles. The first case is the lower limit for the realistic computations, the second case is the upper limit available for the modern computers. That is why only use multiprocessor computer

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systems allow realistic modeling in the mechanics of solids using particles. These methods of modeling in the last decades are being intensively developing abroad, however in Russia it was not possible due to the absence of sufficiently effective computers. Recent development of the multiprocessor computer systems in Russia allows obtaining world competitive results in this area. Usage of multiprocessor systems and development of parallelization technique for the molecular dynamics modeling in mechanics of solids are discussed in the presented lecture.