Crystal plasticity finite element analysis of mechanical behavior of sintered silver nanoparticles

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Abstract

Thanks to the outstanding thermal conductivity and high temperature resistance, silver nanoparticle (AgNP) pastes have become a promising type of die-attach material for electronic packaging structure, especially for high-power electronic devices. The service conditions of die-attach materials become increasingly complex due to the sustainable development of electronic packaging towards high integration and high density, which means that the stress-strain response of die-attach materials must be accurately predicted when it is in use. Considering that the existing macroscopic constitutive model has been incapable of effectively satisfying the needs of microscopic modeling, a framework of crystal plasticity (CP) theory based on mesoscopic mechanics has been established from the dislocation slip mechanism of crystal deformation so as to describe the influence of microstructure evolution on the macro properties of materials. Crystal plastic finite element model (CPFEM) combining finite element analysis and crystal plasticity deformation has been widely adopted along with the unceasing development of finite element technology.

In this study, the simulation of crystal deformation based on the CPFEM is realized in FE analysis software ABAQUS and the constitutive model of mechanical response of sintered AgNP materials is described in order to establish the relationship between meso- and macro-deformation responses of crystal materials of sintered AgNP. Firstly, the framework CP theory is proposed for sintered AgNP, which is realized as a user-defined material model (UMAT) in ABAQUS and a polycrystalline FE model containing sintered AgNPs based on the microscopic characteristics of sintered AgNPs is created combined with Voronoi technology and imported into ABAQUS by script. Subsequently, each grain is randomly assigned with initial orientation and material parameters through Python. The CP parameters for sintered AgNP in the existing literature are referred and further calibrated in this study. As a conventional calibration method, the uniaxial tensile tests of sintered AgNP subjected to different strain rates and temperatures are simulated by the proposed CPFEM. The axial stress-strain curves predicted by CPFEM are found to be consistent with the reported results in the existing literature. According to the predicted stress and strain contours, the distributions of stress and deformation in the polycrystal exhibit great heterogeneity, resulting from the initial orientation of the grains. In other words, the Schmidt factor determined by crystal orientation leads to varying degrees of grain sliding. Generally, the stress concentration is obvious along grain boundaries. Additionally, polycrystalline FE models with different numbers of grains are created by the Voronoi technique to reveal the effect of different average grain sizes on the mechanical behavior of sintered AgNP. On this CPFEM basis, the effect of the initial crystal orientation on the cumulative strain is investigated. Therefore, it can be concluded that the average size of grains and their initial orientations can significantly affect the mechanical behavior of sintered AgNP.

Keywords: Sintered silver nanoparticle; crystal plasticity; constitutive model; finite element method.