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ON THE REPRESENTATIVE VOLUME ELEMENT SIZE FOR QUASI-ISOTROPIC MACROSCOPIC BEHAVIOR OF A Fe-Mn-C STEEL MICROSTRUCTURE SIMULATED BY THE PHASE-FIELD METHOD

Gottfried M. Laschet* and Markus Apel

ACCESS e.V., RWTH Aachen, Intzestrasse 5, D-52072 Aachen, Germany , E-mail:

{g.laschet, m.apel}@access.rwth-aachen.de,

URL: www.access.rwth-aachen.de

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3-D multicomponent multiphase-field simulations of a polycrystal steel microstructure, undergoing austenite to ferrite phase transformation during heat treatment, are time consuming. Mainly the coupled solution of the phase field equations with species diffusion and local stress/strain analysis requires impractical simulation times on multicore CPU's [1]. On the other side, El Houdaigi et al. [2] has shown, via statistical considerations, that the Representative Volume Element (RVE) of a polycrystal must contain at least 445 randomly oriented grains in order to get an isotropic macroscopic behaviour. To reduce this large RVE size for coupled multiphase-field analyses, a new definition of random grain orientations is presented, which for smaller RVEs (less than 100 grains) induces a quasi-isotropic global material behaviour. Indeed, the whole orientation space is divided in sub-regions and the algorithm insures that each sub-region has at least one random orientation. To validate this algorithm effective thermo-elastic and elasto-plastic properties are predicted by computational homogenization for several RVE realizations of the initial austenite microstructure of a Fe-0.17wt%Mn-0.023wt%C steel and their deviation from polycrystal isotropy is determined. These RVEs differ in size and shape and by the number of grains and their orientations. Despite their random nature, periodic boundary conditions are applied there. The convergence of this statistical homogenization analysis allows the definition of a more suitable RVE, presenting a quasi-isotropic global material behaviour. Then, based on this microstructure, the austenite to ferrite phase transformation during cooling of steel disc is calculated at selected locations by the multicomponent multiphase field model [3]. Thermodynamic properties of the individual phases are taken from thermodynamic databases. Temperature and concentration dependent thermo-mechanical properties are specified for each phase [4]. In order to predict effective mechanical properties, geometrical information about the individual grains and their orientation are transferred to the homogenization tool [5]. Effective cubic Young and shear modules and Poisson coefficients are predicted for different ferrite volume fractions as well as effective volumetric eigenstrains and thermal expansion coefficients. At next, by virtual testing, the evolution of the plastic flow curves with the ferrite volume fraction is predicted. Finally, the predicted local effective thermo-mechanical properties are used at the macro-scale to evaluate the stress/strain evolution in the steel disc.

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