
Investigating thermal coupling on diffusive processes in metallic and non-metallic materials

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Abstract

The phenomenon of diffusion, where species move relative to a solid material, is present in various applications such as lithium-ion transport in batteries or oxygen-ion transport in solid oxide fuel cells (1). Since, the properties of materials can change due to a diffusion process, considering metallic materials exposed to hydrogen (2) or polymer materials exposed to moisture (3), precise diffusion models need to be established. Therefore, the thermal influence on a diffusion process is crucial for accurate predictions of material properties. To account for a thermal coupling, a thermo-chemo-mechanical model is developed. The model is embedded within a geometrically linear theory and considers a linear approach for the elastic behavior. A diffusion equation describes the redistribution of species, where the species flux is coupled to the mechanical and thermal fields. An equation of heat conduction is derived accounting for heat production through mechanical dissipation. The model is implemented using a Finite Element approach with the help of the user-defined element (UEL) subroutine of Abaqus, where the displacement field, the chemical potential and the temperature are used as solution variables. The thermal coupling is investigated for metallic and non-metallic materials with a focus on the local temperature evolution as well as on the influence of non-isothermal conditions on the diffusion process. The study outlines the role of thermal coupling while modeling diffusion phenomena.

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