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CZ 結晶成長法におけるシリコン原料装填構造の原料融解および炭素混入過程のモデル化

Dynamic modeling of melting process and carbon contamination in packed Si chunks of Czochralski silicon crystal growth

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Contamination of carbon (C) in Czochralski silicon crystal growth (CZ-Si) mainly originates from carbon monoxide (CO) generation, which is triggered during the heating and melting stages. It is essential to control the CO generation and C incorporation during the melting processes. Poly-Si chunks in the crucible are packed with the porosity due to voids and gaps. The packed Si chunks experience the collapsing and volume shrinking during the melting process. Melting process, as well as the species transport, must be modeled by transient global simulation with the mesh deformation.

Due to the porosity of packing Si chunks, the effective thermal conductivity model proposed by IAEA [1] was applied for the melting process. Original packing volume of Si chunks is shown in Fig.1. And, irregular Si chunks were idealized as identical spheres with voids among them. Once the melting process started from the crucible wall, the packing volume of Si chunks (V_T) decreased due the packing density (≈ 0.7). Volume of the voids (V_P) released as the volume difference (dV) during the melting process, as shown in Fig.2. Mesh deformation rate (dh) is modeled as the function of the released volume of voids (dV), which also results in mesh deformation of the argon gas domain. Transport phenomena of heat and species in CZ-Si growth, besides the accumulation of C in Si feedstock, were predicted within this transient global modeling framework.

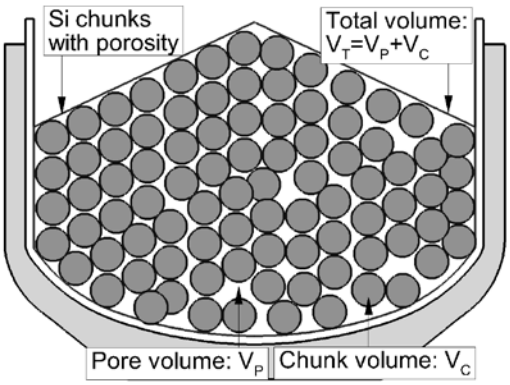

Fig. 1 Idealized packing volume of Si chunks

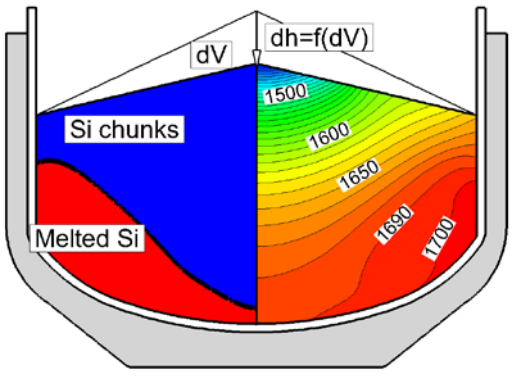

Fig. 2 Intermediate volume of the melting Si

[1] IAEA-TECDOC-1163, 2000, IAEA, Vienna.

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