Mg_2Si crystal growth by the vertical Bridgman method: scale-up and optimization by modeling and growth experiments

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As a low cost and environmentally friendly semiconductor, magnesium silicide (Mg_2Si) has shown potential for the fabrication of infrared detectors and thermoelectric generators. We have grown 1-inch Mg_2Si single crystals by the vertical Bridgman (VB) method using pyrolytic boron nitride (pBN) crucibles coated with boron nitride (BN) [1]. However, there are still two difficulties in scale-up to larger size ingot growth by the VB process. First, Mg_2Si crystal is brittle and has a low fracture toughness, which can cause cracks to form at the local stress concentrations. Second, Mg_2Si ingot has a relatively high thermal expansion coefficient (46.9×10^{-6} K^{-1}) [2]. Thus, annealing from growth to room temperature could activate the small-angle grain boundary or even dislocation cluster generations. To realize the 2-inch Mg_2Si crystal growth, we integrate the growth experiments and transient global simulations to optimize the growth conditions.

A 2-inch Mg_2Si ingot of 25 mm height was grown at the basis of the 1-inch VB crystal growth process. Meanwhile, we build the transient global model to reproduce the entire growing process, as shown in Fig. 1. Besides reproducing the growing process, we must also predict the risk of cracking and dislocation generation, which easily occurs in Mg_2Si ingot growth. Based on the fracture toughness and thermal expansion coefficient of Mg_2Si crystal, we could estimate the critical stress (1.8 MPa) for crack occurrence. The predicted maximum von Mises stress was close to the crucible wall, as shown in Fig. 2 (a). This is consistent with the half slice of the grown crystal that cracked at the periphery (Fig. 2(b)). Based on this validated model, we optimized the hot zone and the annealing recipe to improve the crystal quality. The buffer layer under the crucible and the cooling rate below 8 K/h for annealing were favorable for Mg_2Si crystal growth without cracks and dislocation clusters. The crystal height could also be doubled under the optimized growth conditions according to the simulation and experimental results.

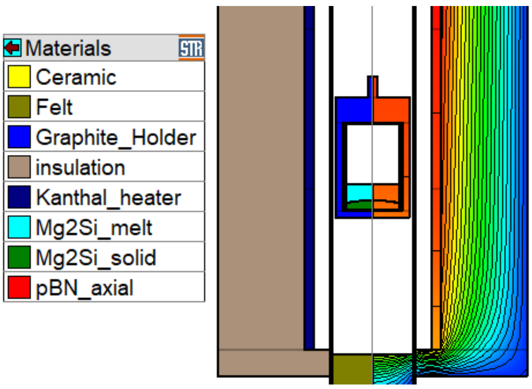

Fig. 1 Global simulation for Mg_2Si crystal growth

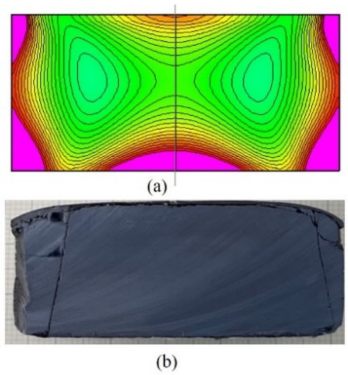

Fig. 2 Cracking prediction and validation

References

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