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On the Generation Mechanism of Large-size CaO•Al2O3 Inclusions in Die Steel during the Electroslag Remelting Process: at Atomic Scale

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It is generally believed that electroslag remelting can effectively reduce the number of large-size nonmetallic inclusions in steel and improve solidification structure, thus electroslag remelting (ESR) has become the main method to produce high quality die steel. However, large-size inclusions (D and Ds type) have been aperiodically detected in the production-scale ESR die steels. The detection results indicate that majority large inclusions are CaO•Al2O3 inclusions and reducing calcium content in die steel is important to control D and Ds inclusions. In this work, we have focused on the generation mechanism of large-size CaO•Al2O3 inclusions in die steel during the electroslag remelting process. It was proposed that the concentration of free Ca2 + ions (calcium activity) in ESR slags was the key parameter that determines the calcium content and CaO•Al2O3 inclusions in ESR die steels. Considering various CaF2-containing slags (CaF2-CaO-Al2O3-SiO2-MgO), the bond configuration and mean square displacement of Ca2+ ions were studied based on molecular dynamics simulation. Combined with ion and molecular coexistence theory (IMCT), we established a model to calculate the calcium activity. The model indicated that CaF2 component in slags significantly determine the calcium activity since Ca2+ ions provided by CaF2 could move freely and hard to be incorporated into complex molecular cluster. A novel ESR slag with low CaF2 content has been developed and applied in the industrial production of die steel, calcium content and large-size CaO•Al2O3 inclusions been successfully reduced, validating the reliability of the theoretical analysis. This work has established the intrinsic relationship between large-size inclusion in ESR die steel and microscopic atomic structure of ESR slag. This is of great significance to optimize the ESR slag composition to improve the metallurgy quality of ESR die steels.

Speaker Country

China

Primary authors: Prof. ZHOUHUA , Jiang (Northeastern University); Dr TIAN, Jialong (Northeastern University); Mr LI, Diyue (Northeastern University)

Presenter: Dr TIAN, Jialong (Northeastern University)

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