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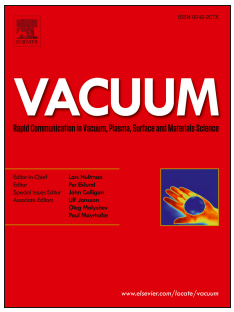

Prediction and application of Si-Ca and Si-Ca-Fe alloy solutions by co-existence theory model

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Prediction and application of Si-Ca and Si-Ca-Fe alloy solutions by co-existence theory model

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Abstract: Based on the atom and molecule co-existence theory (AMCT), the activity models of Si-Ca and Si-Ca-Fe alloy solutions were established. The self-interaction coefficient and infinitely diluted activity coefficient of Ca, along with the interaction coefficient of Ca-Fe in silicon alloy solutions, were calculated at a temperature range of 1723-1873K. The calculated data agree well with the experimental values and indicate that the atom and molecule co-existence theory is reliable for predicting the activity of Si-Ca and Si-Ca-Fe solutions. In addition, an iso-activity phase diagram of Si-Ca-Fe solution at 1723 K was plotted. The established activity model of Si-Ca-Fe shows that the activities of $CaSi_2$ and $FeSi_2$ in silicon solution are high. The activities of $CaSi_2$ and $FeSi_2$ are equal at x_{Ca}/x_{Fe}=1.1. The activity of $CaSi_2$ is 9.91 times greater than that of $FeSi_2$ at x_{Ca}/x_{Fe}=10. The effect of x_{Ca}/x_{Fe} on acid leaching was further discussed based on thermodynamics.

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