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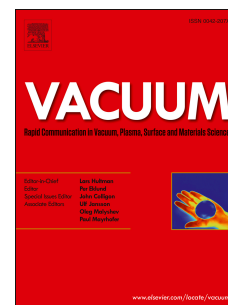
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Prediction and application of Si-Ca and Si-Ca-Fe alloy solutions by co-existence theory model

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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 $x_{\text{Ca}}/x_{\text{Fe}}=1.1$. The activity of CaSi_2 is 9.91 times greater than that of FeSi_2 at $x_{\text{Ca}}/x_{\text{Fe}}=10$. The effect of $x_{\text{Ca}}/x_{\text{Fe}}$ on acid leaching was further discussed based on thermodynamics.

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