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酸性NaF-AlF3熔盐离子结构的Raman光谱

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摘 要：采用紫外激光Raman光谱，在封闭样品池中研究不同分子比的酸性NaF-AlF_3熔盐的离子结构。结果表明：当电解质分子比为1时，熔盐中的铝氟离子团只以 的形式存在，而对于分子比大于1的酸性电解质，熔盐中有 和 两种铝氟离子团形式；随着温度的增加， 离子团的“寿命”越来越短，而且 特征波段峰的峰位随分子比的增加而发生红移，温度对 的“寿命”影响不大。Raman光谱的定量分析表明，在测量的熔盐配重分数区间内，温度对于熔盐中各离子摩尔分数的影响不大，而且F^-含量很小，当NaF的配重摩尔分数为0.60时， 的摩尔分数在0.75左右，的摩尔分数仅约为0.25；当NaF的配重摩尔分数增至0.71时， 的摩尔分数降为0.25左右， 增为约0.75。

关键字： NaF-AlF3熔盐；离子结构；铝氟离子团；Raman光谱

Raman spectra of ionic structure for acidic NaF-AlF3 melts

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Abstract: The ionic structure of acidic NaF-AlF3 melts with different cryolite ratios(CR) was studied in the sealed sample cell by UV laser Raman spectra. The results show that only one kind of Al-F complex ions— exists in the melts with CR=1; However, two kinds of Al-F complex ions, and exist in the acidic melts with CR more than 1. The “lifetime” of decreases increasing with temperature and the main Raman band wavenumber of shows red-shift with increasing CR values, but temperature has little effect on the “lifetime” of . Quantitative analysis of measured Raman spectra results show that in the measuring temperature and weighted-in mole fraction range, temperature has little influence on the mole fraction of anions in the melts, and the content of F− is low. The mole fraction of is about 0.75 for the melts whose weighted-in mole fraction of NaF is 0.6, but that of is about 0.25. When the weighted-in mole fraction of NaF increases to 0.71, the mole fraction of decreases to 0.25 while that of increases to 0.75.

Key words: NaF-AlF3 melts; ionic structure; Al-F complex ions; Raman spectra

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