

Computer simulations of double-doped LiNbO₃

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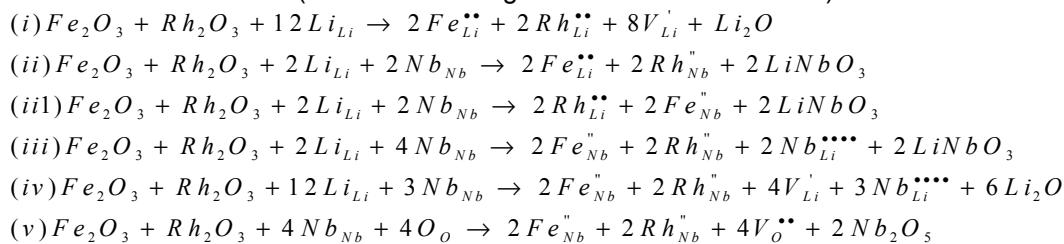
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Abstract- Lithium niobate, LiNbO₃, is one of the most important synthetic crystal with good electro-optic, acousto-optic, elasto-optic, piezoelectric and nonlinear properties[1]. Computer modelling provides a useful means of determining the properties of the material, including its defect chemistry, and the effect of doping on the structure. The next step of the work is to analyse the doubly doped in LiNbO₃.

Photorefractive lithium niobate (LiNbO₃) crystals have been extensively investigated as attractive holographic recording materials because of their photorefractive properties and availability in large size and good quality[1]. The experimental results show that nonvolatile holographic recording has been achieved in differently doped LiNbO₃ crystals, such as LiNbO₃:Fe,Cu, LiNbO₃:Fe,Ni, LiNbO₃:Ce,Cu, LiNbO₃:Ce,Mn and LiNbO₃:Fe,Rh. Computer modelling provides a useful means of determining the properties of the material, including its defect chemistry, and the effect of doping on the structure. Previous papers have presented a new potential model for the material [2] and reported the doping of structure by rare earth ions [3]. Double-doped LiNbO₃ is important in many applications. Zn:Fe:LiNbO₃ were shown to have improved holographic properties compared with crystals of Fe/LiNbO₃ [4]. A comprehensive study by McMillen and co-authors showed that the ability to record a hologram, the stability of the system and the scattering of light is strongly influenced by co-doping in LiNbO₃ [5].

This work reports a computational study of the doping of LiNbO₃ by Fe and Cu, Fe and Ni, Ce and Cu, Ce and Mn and Fe and Rh. Solution energies are calculated for doping with this ion, which enable predictions of mechanisms in the material. The calculations were performed using the GULP code. The LiNbO₃:Fe,Rh dopant ions can potentially be incorporated at either the Li⁺, or the Nb⁵⁺ site, and the following possible defect reactions were considered (the standard Kroger-Vink notation was used):



The first equation represents a possible mechanism of incorporation of the Fe³⁺ and Rh³⁺ ions at the Li⁺ site with charge compensation by Li vacancies. The second reaction represents the incorporation of Fe³⁺ and Rh³⁺ at both Li and Nb sites. Reaction iii and iv represents two possible schemes for incorporation of the dopants at the Nb site with charge compensation by Nb in the Li site (reaction iii) or Li vacancies (reaction iv). Reaction v represents the incorporation of the dopants at the Nb site with charge compensation by an oxygen vacancy. All solution energies are shown in table 1. The results in table 1 are consistent with the previous work on rare earth doping [1] and the Fe³⁺ and Rh³⁺ are likely to simultaneously occupy both the Li and Nb sites, thus generating Fe³⁺ and Rh³⁺ ions in two different site symmetries.

Table 1. Solution energies (per dopant ion)(eV)

Defect	(i)		(ii)		(iii)		(iv)		(v)			
	0	293	0	293	0	293	0	293	0	293		
Fe,Rh	4.51	4.76	1.11	1.07	1.20	1.22	2.80	2.68	8.20	9.12	3.33	3.48

References

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