

Structural Study of Liquid Lithium Niobate by Neutron Diffraction

Role of the Li Atom in the Clustering Near Solidification

P. Andonov, H. E. Fischer^{a,*}, P. Palleau^a, and S. Kimura^b

CNRS-Laboratoire de Magnétisme et d'Optique de Versailles, Université de Versailles avenue des Etats-Unis Bat. Fermat, 78305 Versailles Cedex, France

^a Institut Laue-Langevin, 156 X centre de tri, 38042 Grenoble Cedex, France

^b National Institute for Research in Inorganic Materials, I-I Namiki, Tsukuba-shi, Ibaraki 305, Japan

* Current address: L.U.R.E. Bat. 209 d, Boite postale 34, Centre Universitaire Paris-Sud, 91898 Orsay Cedex, France

Reprint requests to Mme. P.A; Fax: (1) 39 254 652; E-mail: lmov@physique.uvsq.fr

Z. Naturforsch. **56a**, 395–406 (2001); received February 12, 2001

The structure of liquid LiNbO_3 has been investigated by neutron diffraction using samples with different isotopic composition of lithium. The intensity scattered by these samples has been measured for momentum transfers $0.4 \text{ \AA}^{-1} < Q < 17.1 \text{ \AA}^{-1}$ and temperatures $1600 \text{ K} > T > 1500 \text{ K}$, which include the undercooling domain. From an analysis of the correlation functions $G_{ij}(r)$ of the atomic pairs Li–Li, Li–Nb, Li–O and their structural evolutions, given by $\Delta G_{i-j}(r) = G_{i-j}(r)_{1500} - G_{i-j}(r)_{1550}$ made with reference to the crystalline LiNbO_3 ferroelectric structure, it was possible to confirm a local ordering similar to that of the crystal. The presence of clusters (groupings of NbO_3 octahedra) is confirmed. Both regular and irregular NbO_6 octahedra are observed in the liquid near solidification. With its high mobility in the melt, the Li atom plays an important role in the clustering: the Li–O and Li–Nb bonds make possible the staking of four octahedra groups into clusters of eight octahedra or more. The Li–Li bonds join these groups. The diameter of the clusters is a least 22 \AA in the undercooling regime.

Key words: Structure of Liquids; Neutron Scattering; Atomic Clusters; Liquid Lithium Niobate.