The Canadian Mineralogist
Vol. 38, pp. 183-189 (2000)

A SINGLE-CRYSTAL NEUTRON-DIFFRACTION INVESTIGATION OF DIOPSIDE AT 10 K

MAURO PRENCIPE AND MARIO TRIBAUDINO

Dipartimento di Scienze Mineralogiche e Petrologiche, Università di Torino, Via Valperga Caluso 35, I-10125 Torino, Italy

ALESSANDRO PAVESE

Dipartimento di Scienze della Terra, Università di Milano, Via Botticelli 23, I-20133 Milano, Italy

ANDREAS HOSER AND MANFRED REEHUIS

Hahn-Meitner-Institut Berlin, Glienicker Strasse 100, D-14109 Berlin, Germany

Abstract

Single-crystal neutron-diffraction data, collected at 10 K on a natural sample of diopside, provided a structure that refined to $R = 4.5\%$ for 415 independent reflections. The structure refinement showed significant reduction of the $M(2)$–O(3C2),(3D2) bond lengths, resulting in a more regular $M(2)$ polyhedron than at higher temperatures. A significant *zero-point* contribution to the atomic displacement parameters (*ADP*) was found. On average, it accounts for the 35% of the room-temperature determination. Such results confirm previous predictions based on lattice-dynamics calculations.

Keywords: diopside, neutron diffraction, low-temperature structure, zero-point motion.

Sommaire

Des données en diffraction neutronique, prélevées à 10 K sur un cristal unique de diopside naturel, ont mené à une structure affinée jusqu'à un résidu R de 4.5% en utilisant 415 réflexions indépendantes. L'affinement de la structure indique une réduction importante de la longueur des liaisons $M(2)$–O(3C2),(3D2) et, par conséquent, un polyèdre $M(2)$ plus régulier qu'aux températures plus élevées. Le mouvement des atomes au point zéro contribuerait de façon importante aux paramètres décrivant les déplacements atomiques. Par exemple, en moyenne, ce mouvement rend compte de 35% des valeurs établies à température ambiante. Ces résultats confirment les prédictions antérieures fondées sur les calculs de la dynamique du réseau.

Mots-clés: diopside, diffraction neutronique, structure à basse température, mouvements au point zéro.

Introduction

Clinopyroxenes are important rock-forming minerals. The reference clinopyroxene end-member is diopside ($CaMgSi_2O_6$); in fact, the composition of natural clinopyroxenes, for example augite, can be derived by solid solution in the cation sites of diopside. Therefore, several structural investigations have been performed on both natural and synthetic diopside to clarify its structural features in relation to those of other clinopyroxenes at room (Clark *et al.* 1969, Bruno *et al.* 1982) and non-ambient conditions (high pressure: Levien & Prewitt 1981, Zhang *et al.* 1997; high temperature: Cameron *et al.* 1973, Finger & Ohashi 1976). The main result of the cited papers was a description of the evolution of the average bond-lengths and distortion of polyhedra as a function of temperature (T), pressure (P) and composition.

At present, no data exist on the diopside structure at T close to 0 K; the purpose of this work is to provide structural data on diopside at low temperature. A refinement at low T is of interest (i) to show the structural variations that occur at low T with respect to the room-temperature and high-temperature data (Cameron *et al.* 1973, Finger *et al.* 1976); (ii) to evaluate experimentally the extent of *zero-point motion* in diopside and to compare these results with theoretical predictions provided by lattice dynamics (Pilati *et al.* 1996). Experi-

E-mail addresses: prencipe@dsmp.unito.it, triba@dsmp.unito.it, pavese@p8000.terra.unimi.it, hoser@hmi.de, reehuis@hmi.de