Ni$_3$Se$_2$ has a complex heazlewoodite-type structure. In heazlewoodite, in addition to the Ni-S bond, the Ni-Ni bond plays an important role in structural stabilization and physical properties. The crystal structure of Ni$_3$Se$_2$ [rhombohedral, space group $R\bar{3}2$, $a = 6.02813(13)$ Å, $c = 7.24883(16)$ Å, $Z = 3$] was analysed by single-crystal X-ray diffraction and refined to yield $R$ value of 0.020 for 117 unique reflections. $R\bar{3}2$ is a Sohncke type of space group where enantiomeric structures can exist; the single-domain structure obtained by the refinement was confirmed to be correct by a Flack parameter of -0.05(2). The existence of Ni-Ni bonds was confirmed in the structure (Figure 1), in addition to the Ni-Se bonds [1]. The Debye temperature, $\theta_D$, for each site can be estimated using the dynamic component in Debye-Waller factor. The $\theta_D$ is one of the indices as a physical quantity that can be compared among materials with different compositions. The phonon density of states estimated from lattice dynamics calculations coincides well with the observed $\theta_D$ values. The Debye temperatures estimated from observed Debye-Waller factors for Ni and Se in Ni$_3$Se$_2$ were 322 K and 298 K, respectively [1]. Those for Ni and Se in NiSe were 246 K and 241 K, and for Ni and Sb in NiSb were 275 K and 206 K, respectively. The Debye temperatures of cations are higher than those of anions in these compounds and a correlation between cation-anion distances and Debye temperatures was confirmed. In contrast, the Debye temperatures of cations are significantly lower than those of anions in most Ni sulphides. The Debye temperatures of the heazlewoodite-type structures are on the same trend as other Ni chalcogenides.

Keywords: Ni$_3$Se$_2$, Ni chalcogenides, Debye temperatures, single crystal diffraction

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