American Mineralogist, Volume 84, pages 669–676, 1999

Toward the crystal structure of nagyagite, $[Pb(Pb,Sb)S_2][(Au,Te)]$

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ABSTRACT

Synthetic nagyagite was grown from a melt as part of a search for materials with high-temperature superconductivity. Electron microprobe analyses of synthetic nagyagite and of nagyagite from the type locality Nagyág, Transylvania (now Săcărîmb, Romania) agree with data from literature. The crystal chemical formula $[Pb(Pb,Sb)S_2][(Au,Te)]$ was derived from crystal structure investigations. Nagyagite is monoclinic pseudotetragonal. The average crystal structure was determined from both synthetic and natural samples and was refined from the synthetic material to $R = 0.045$ for 657 single-crystal X-ray data: space group $P2_1/m$, $a = 4.220(1)$ Å, $b = 4.176(1)$ Å, $c = 15.119(3)$ Å, $\beta = 95.42(3)°$, and $Z = 2$. Nagyagite features a pronounced layer structure: slices of a two slabs thick SnS-archetype with formula $Pb(Pb,Sb)S_2$ parallel to (001) have a thickness of 9.15 Å. Te and Au form a planar pseudo-square net that is sandwiched between the SnS-archetype layers; it is assumed that planar $Au^{[4Te]}Te_4$ configurations are edge connected to chains and that Te atoms are in a zigzag arrangement. Ordering within the SnS-archetype and gold-tellurium layers, intense twinning and/or stacking variants are responsible for the often observed superstructure reflections. For buckhornite, $[(Pb_2Bi)_{\Sigma 3}S_3][(AuTe_2)_{\Sigma 3}]$, a structure model is proposed considering a homologous series with nagyagite, $[(Pb_3(Pb,Sb)_3)_{\Sigma 6}S_6][(Au,Te)_3]$.