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The role of silver on the stabilization of the incommensurately modulated structure in calaverite, $AuTe_2$

Luca Bindi,[1,*] Alla Arakcheeva,[2] and Gervais Chapuis[2]

[1]Museo di Storia Naturale, Sezione di Mineralogia, Università di Firenze, Via La Pira 4, I-50121 Firenze, Italy
[2]École Polytechnique Fédérale de Lausanne, Laboratoire de Cristallographie, BSP, CH-1015 Lausanne, Switzerland

Abstract

Structural investigations of several minerals belonging to the calaverite group with composition $Au_{1-x}Ag_xTe_2$ (x = 0.00, 0.02, 0.05, 0.09, 0.19, and 0.33) indicate that Ag is randomly distributed on the Au sites. This suppresses the valence fluctuation of Au and, therefore, the structure modulations. The results are compared with the previously published incommensurately modulated structure of calaverite, $Au_{0.9}Ag_{0.1}Te_2$, which is characterized by valence fluctuations of Au reinforced by an ordered distribution of Ag. The (3+1)-dimensional calaverite structure type is able to reproduce both (3+1)D and 3D related structures with the general formula AB_2 (A = Au, Ag, Cu, Nb, Ta; B = Te).

Keywords: Calaverite, modulated structure, valence fluctuations, krennerite