

## The new mineral crowningshieldite: A high-temperature NiS polymorph found in a type IIa diamond from the Letseng mine, Lesotho

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### ABSTRACT

Crowningshieldite is the natural analog of the synthetic compound  $\alpha$ -NiS. It has a NiAs-type structure and is the high-temperature polymorph relative to millerite ( $\beta$ -NiS), with an inversion temperature of 379 °C. Crowningshieldite is hexagonal, space group  $P6_3/mmc$ , with  $a = 3.44(1)$  Å,  $c = 5.36(1)$  Å,  $V = 55.0(2)$  Å<sup>3</sup>, and  $Z = 2$ . It has an empirical formula  $(\text{Ni}_{0.90}\text{Fe}_{0.10})\text{S}$  and  $d_{\text{calc}} = 5.47(1)$  g/cm<sup>3</sup>. The five strongest lines in the powder X-ray diffraction data are [ $d_{\text{meas}}$  in angstroms ( $l$ ) ( $hkl$ ): 1.992 (100) (102), 1.718 (55) (110), 2.978 (53) (100), 2.608 (35) (101), and 1.304 (17) (202). Crowningshieldite was found as part of a multiphase inclusion in a gem-quality, colorless, type IIa (containing less than ~5 ppm N) diamond from the Letseng mine, Lesotho. The inclusion contains crowningshieldite along with magnetite-magnesioferrite, hematite, and graphite. A fracture was observed that extended from the inclusion to the diamond exterior, meaning that fluids, possibly kimberlite-related, could have penetrated into this fracture and altered the inclusion. Originally, the inclusion might have been a more reduced, metallic Fe-Ni-C-S mixture made up of cohenite, Fe-Ni alloy, and pyrrhotite, akin to the other fracture-free, pristine inclusions within the same diamond. Such metallic Fe-Ni-C-S primary inclusions are a notable recurring feature of similar type IIa diamonds from Letseng and elsewhere that have been shown to originate from the sublithospheric mantle.

The discovery of crowningshieldite confirms that the  $\alpha$ -NiS polymorph occurs in nature. In this case, the reason for its preservation is unclear, but the relatively iron-rich composition [ $\text{Fe}/(\text{Fe}+\text{Ni}) = 0.1$ ] or the confining pressure of the diamond host are potential factors impeding its transformation to millerite. The new mineral name honors G. Robert Crowningshield (1919–2006) (IMA2018-072).

**Keywords:** Crowningshieldite,  $\alpha$ -NiS, inclusion, type IIa diamond, Letseng