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Determination of the structure and the properties of a new nickel nitride

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Contrary to Fe, Co or Cu nitrides, the Ni ones are scarcely studied. Thus, the binary Ni-N system is not well defined. It contains a stable hexagonal phase that exhibits a Ni_3N formula. Although another nitride (Ni_2N) has been also reported, the structure and the properties of this material are not clearly detailed in the literature.

Nickel nitride thin films have been deposited at room temperature on glass and silicon substrates by reactive sputtering of a Ni target in various Ar- N_2 atmospheres. The increase of the N_2 partial pressure allows the deposition of either pure Ni_3N or Ni_2N films. Biphased films can be also deposited with the use of a N_2 flow rate ranging between those necessary to deposit single phase. Electron probe microanalysis has been used to determine the Ni / N atomic ratio in as-deposited films. Ni_2N films exhibit a preferential orientation in the [110] direction. Cumulative X-ray diffractogram obtained at various θ angles has been used to show that Ni_2N crystallizes with a primitive tetragonal unit cell (space group: P4/mmm). Full profile refinement using a Rietveld method confirmed the atomic arrangement proposed by ab initio calculation using USPEX code. Nickel atoms are located at (0,0,0) and (1/2,1/2,1/2) while nitrogen ones are located at (1/2,1/2,0).

Ni_2N films have been annealed from 100 to 300 °C. XRD analyses of films annealed at 100 and 150 °C show a slight shift of the Ni_2N (110) diffraction peak position due to a progressive denitridation. In addition to Ni_2N , Ni_3N is evidenced after annealing at 200 and 250 °C. Finally, metallic nickel is observed after annealing at 300 °C. The electrical properties of Ni_2N films have been determined and compared to those of Ni_3N .

Keywords

Structure determination

Ab initio calculation

Nickel nitride

Thermal stability

Electrical properties