

Accepted Manuscript

Study of the iron nitride FeN into the megabar regime

Dominique Laniel, Agnès Dewaele, Simone Anzellini, Nicolas Guignot



PII: S0925-8388(17)33703-9

DOI: [10.1016/j.jallcom.2017.10.267](https://doi.org/10.1016/j.jallcom.2017.10.267)

Reference: JALCOM 43664

To appear in: *Journal of Alloys and Compounds*

Received Date: 12 July 2017

Revised Date: 5 October 2017

Accepted Date: 29 October 2017

Please cite this article as: D. Laniel, Agnès Dewaele, S. Anzellini, N. Guignot, Study of the iron nitride FeN into the megabar regime, *Journal of Alloys and Compounds* (2017), doi: 10.1016/j.jallcom.2017.10.267.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Study of the iron nitride FeN into the megabar regime

Dominique Laniel,^{1*} Agnès Dewaele,¹ Simone Anzellini,² Nicolas Guignot³

¹CEA, DAM, DIF, F-91297 Arpajon, France

²Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK

³Synchrotron SOLEIL, St-Aubin 91192, France

Abstract

In this work, the nitrogen-rich portion of the Fe-N binary phase diagram is investigated up to 128 GPa. The samples, largely in excess of nitrogen, were laser-heated in diamond anvil cells to temperatures of 1500–2500 K at regular pressure intervals to help in crossing possible activation barriers towards the more stable phase. Three Fe-N compounds: ZnS-type FeN, Fe₂N and NiAs-type FeN, are characterized by powder X-ray diffraction and their observed stability domain reported. Below 12.5 GPa, orthorhombic Fe₂N is found to be the energetically-favored compound while NiAs-FeN becomes stable above 17.7 GPa. Energy-dispersive X-ray spectroscopy measurements and a Rietveld refinement confirmed the stoichiometry and structure of the recovered NiAs-FeN sample. A precise determination of its bulk modulus ($K_0 = 200(5)$ GPa) as well as its pressure derivative ($K_0' = 5.3(2)$) is obtained and, based on its unit cell axial ratio evolution, the NiAs-FeN compound appears to decrease in ionicity concomitantly with pressure. Within the pressure-temperature conditions reached here, the predicted iron pernitride FeN₂ is not observed.

keywords: high pressure, chemical synthesis, X-ray diffraction, synchrotron radiation, crystal structure and symmetry

1. Introduction

Transition metal nitrides are known to be a large group of industrially relevant compounds with outstanding physical properties, specifically regarding their high hardness, high bulk modulus and refractory, superconducting as well as catalytic properties.^{1,2} Of particular interest are the nitrogen-rich metal pernitrides, composed of charged single-bonded N-N dimers.³ Their unique mechanical and electronic properties are thought to originate from the significant transition metal-nitrogen charge transfer and the nature of the N-N bond.^{4–6} With the notable exception of TiN₂,⁶ synthesized transition metal pernitrides (OsN₂, IrN₂, PtN₂, RuN₂, RhN₂, PdN₂)^{4,5,7–10} form N-N connected MN₆ octahedrons (M standing for metal) and exhibit a variety of electronic structures corresponding to that of a metal, semiconductor and insulator. Furthermore, they are known for their ultrahigh-incompressibility, similar to that of cubic boron nitride.¹¹

Download English Version:

<https://daneshyari.com/en/article/7994875>

Download Persian Version:

<https://daneshyari.com/article/7994875>

[Daneshyari.com](https://daneshyari.com)