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Controlling Dimensionality in the Ni−Bi System with Pressure

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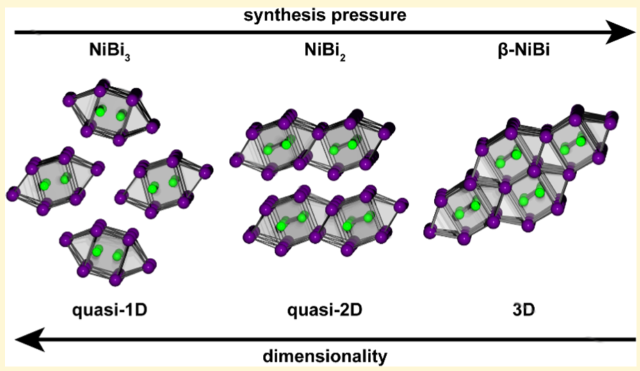
Supporting Information



ABSTRACT: The discovery of new layered materials is crucial for the development of novel low-dimensional materials. Here, we report in situ high-pressure studies of the quasi-one-dimensional (1D) material $NiBi_3$, revealing the formation of a new layered intermetallic phase, $NiBi_2$. In situ diffraction data enabled us to solve the structure of $NiBi_2$, which crystallizes in the same structure type as $PdBi_2$, adding to a growing number of examples in which first-row transition-metal binary systems form structures at high pressure comparable to the ambient-pressure structures of their second-row congeners. Based upon the diamond anvil cell reactions, we initiated scale-up reactions in a multianvil press and isolated bulk $NiBi_2$. Isolating a bulk sample enabled us to evaluate prior theoretical predictions of phase stability for $NiBi_2$. Our findings of metastability within this phase are contrary to previous predictions, recommending continuing research into this phase. The dimensionality of the building units seems to vary as a function of synthesis pressure in the Ni−Bi system, being quasi-1D at ambient pressures ($NiBi_3$), quasi-two-dimensional at ∼14 GPa ($NiBi_2$), and three-dimensional at ∼39 GPa (β-NiBi). This observation represents the first demonstration of dimensionality control in a binary intermetallic system via application of pressure.

The discovery and characterization of new two-dimensional (2D) materials is at the forefront of contemporary physics and materials science.[1,2] The dimensional reduction from bulk to 2D transforms the electronic structure of these materials, resulting in unexpected physical and electronic properties including unusual magnetooptical effects, superconductivity, and unexpectedly high electron mobilities.[3−5] Discovering new synthetic approaches to create layered structures amenable to exfoliation is the key initial step to accessing novel 2D materials.[6,7] One initially counterintuitive approach is the application of high pressure to increase the dimensionality of one-dimensional (1D) compounds to create layered systems. Our specific target of interest was the Ni−Bi binary system, which contains two thermodynamically stable superconducting intermetallic compounds: α-NiBi (T_c = 4.25 K) and quasi-1D $NiBi_3$ (T_c = 4.06 K).[8−12] We sought to compress the quasi-1D $NiBi_3$ to create a new, layered Ni−Bi intermetallic compound. Toward that end we harnessed the transparency of diamond to probe the formation of new phases in the Ni−Bi system within a diamond anvil cell (DAC). We can use powder X-ray diffraction (PXRD) to observe the reaction progression and thereby establish the reaction conditions required for scale-up.

Herein, we report the discovery of the new layered binary intermetallic compound, $NiBi_2$, synthesized at ∼14 GPa and ∼675 °C from a pure sample of $NiBi_3$. $NiBi_2$ is composed of Bi−Ni−Bi layers that stack along the crystallographic *a*-axis (Figure 1). Intriguingly, the basic structural unit comprising the layers is identical to that found in the quasi-1D $NiBi_3$ compound as well as the compact high-pressure β-NiBi phase.[13] To the best of our knowledge, this is the first example in a binary intermetallic system where the underlying coordination geometry of the transition metal is maintained, whereas the dimensionality of the structure is controlled by pressure from quasi-1D to quasi-2D. The new intermetallic is pressure-quenchable, and preliminary magnetic measurements suggest a potential superconducting transition at T_c ∼ 4.2 K. The discovery of this compound illuminates the layered structures achievable at high pressure.

In situ structural and spectroscopic monitoring of reactions during pressurization and heating were performed in a laser-heated diamond anvil cell (LH-DAC).[14] A polycrystalline

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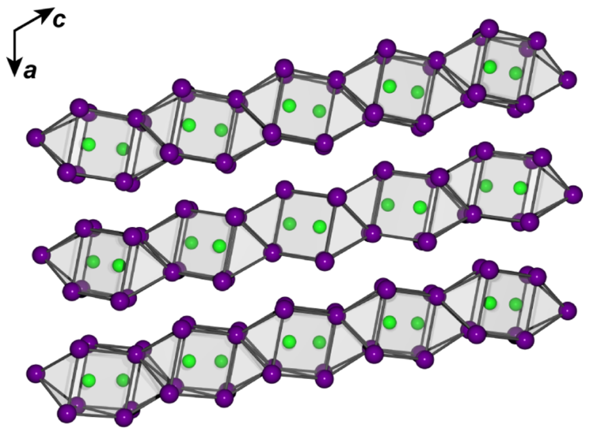

Figure 1. Structure of $NiBi_2$ emphasizing the layered nature of the material. Violet and green spheres represent Bi and Ni, respectively.

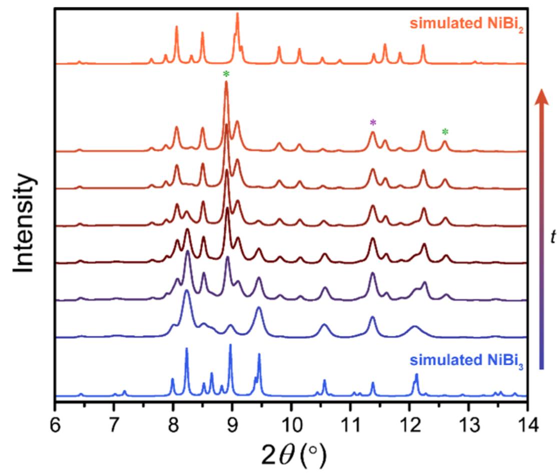

Figure 2. Background-subtracted in situ powder X-ray diffraction patterns taken during heating of $NiBi_3$ in a LH-DAC at 14.8(1) GPa and ∼675 °C (λ = 0.406626 Å). During heating, $NiBi_3$ converts to $NiBi_2$ and elemental Bi (denoted by green asterisks) and the pressure drops slightly to 14.5(1) GPa. MgO is denoted by the violet asterisk. The top and bottom patterns are simulated powder patterns of $NiBi_2$ and $NiBi_3$, respectively.

powder of $NiBi_3$ was pressed into a flake and placed into the cell between two discs of single-crystal MgO, which were used as a thermal insulator, pressure-transmitting medium, and in situ pressure calibrant.[15] Heating within the cell was achieved using two infrared lasers, each focused to a full width at half maximum (FWHM) of ∼40 μm. We acquired in situ synchrotron powder X-ray diffraction (PXRD) data continuously during heating, using 30 keV radiation focused to a FWHM of ∼10 μm.[14] All in situ data were acquired at 16-ID-B, HPCAT at the Advanced Photon Source (APS).

To search for new low-dimensional intermetallic compounds, we pressurized the sample of $NiBi_3$ to ∼14.8(1) GPa. The PXRD pattern before laser heating consisted of broad peaks corresponding to $NiBi_3$ and MgO. The broadness of the peaks is due to the microscopic strain induced by non-hydrostatic compression in the solid pressure-transmitting medium, MgO. As the temperature was increased, the peaks sharpened due to thermal annealing, which relieves the strain in the $NiBi_3$ powder. Upon heating to approximately 675 °C, new Bragg peaks began to appear in the PXRD pattern concomitant with a decrease in intensity of the peaks corresponding to $NiBi_3$, suggesting the synthesis of a new intermetallic phase (Figure 2). After approximately 2 min at this temperature, the peaks corresponding to $NiBi_3$ were no longer observable, and the pressure within the cell had gradually decreased to 14.5(1) GPa. Since the diffraction pattern remained invariant, we turned off the laser to thermally quench the reaction. After quenching the reaction, three phases were present in the PXRD pattern: the unidentified phase, elemental Bi(V), and MgO. The new Bragg reflections corresponded neither to the known structures of α-NiBi, β-NiBi, face-centered cubic-Ni, nor any other polymorphs of elemental bismuth, indicating that a new compound had been accessed through high-PT synthesis. Further, the generation of elemental Bi(V) during heating suggested that the new intermetallic phase was formed by a release of bismuth from the $NiBi_3$ structure.

The high quality of the PXRD data enabled structural identification of the new phase with the aid of a structural model. We initially modeled the known MgO and Bi(V) phases, enabling assignment of the Bragg peaks corresponding to the new phase. These peaks were indexed to the monoclinic space group $C2/m$ with lattice parameters a = 12.1135(3) Å, b = 3.83754(9) Å, c = 5.2749(2) Å, and β = 100.909(3)° at a pressure of 14.1(1) GPa using the TOPAS software package.[16]

We searched the Inorganic Crystal Structure Database (ICSD)[17] for known structures with similar chemistry, symmetry, and lattice parameters and determined that the new phase could be modeled in the CeAlCo structure type with Ni residing on the Co site and Bi on both the Ce and Al sites.[18] In the refined structure of $NiBi_2$ in the CeAlCo structure type, the Ni atoms are coordinated by seven Bi atoms and two Ni atoms, in a tricapped trigonal prismatic geometry (Figure S3). Excluding the Ni atoms, the coordination of the Bi around the central Ni atom is a monocapped trigonal prism (Figure S3). These polyhedra are rectangle-face-sharing to form prism rods and enable Ni−Ni bonding in the form of a zigzag chain. These prism rods are triangle-face-sharing to form a layered structure (Figure 1). Further inspection of the ICSD revealed that the chemically similar superconducting intermetallic mineral froodite, or $PdBi_2$ (T_c = 1.7 K), crystallizes in this same structure type.[19] This finding is in accordance with a guideline to predict high-pressure structural changes formulated by Prewitt and Downs: "elements behave at high pressure like the elements below them in the periodic table at lower pressure."[20] The ambient-pressure stability of $PdBi_2$ and high-pressure stability of $NiBi_2$ suggest that this approach can be extended to binary systems. In this case, the first-row transition-metal binary compound $NiBi_2$ behaves at high pressure like the second-row binary intermetallic $PdBi_2$ behaves at ambient conditions. This type of behavior is also observed for the high-pressure phase $CoBi_3$, which crystallizes in the same space group as ambient-stable $RhBi_3$.[21,22] The extension of this rule could have important implications for other transition-metal main-group binary systems where the second-row compound exists, but no first-row analogue is known. Using this guideline as a predication pathway enables the selection of stoichiometric ratios of elements for high-pressure synthesis and hints at pathways to isolate desired structure types with different elements.

Further consideration of the structure of $NiBi_2$ reveals that it is the quasi-2D analogue of the quasi-1D $RhBi_3$ structure type that the thermodynamically stable precursor, $NiBi_3$, crystallizes in (Figure 3).[11] Both structures are comprised of Ni-centered

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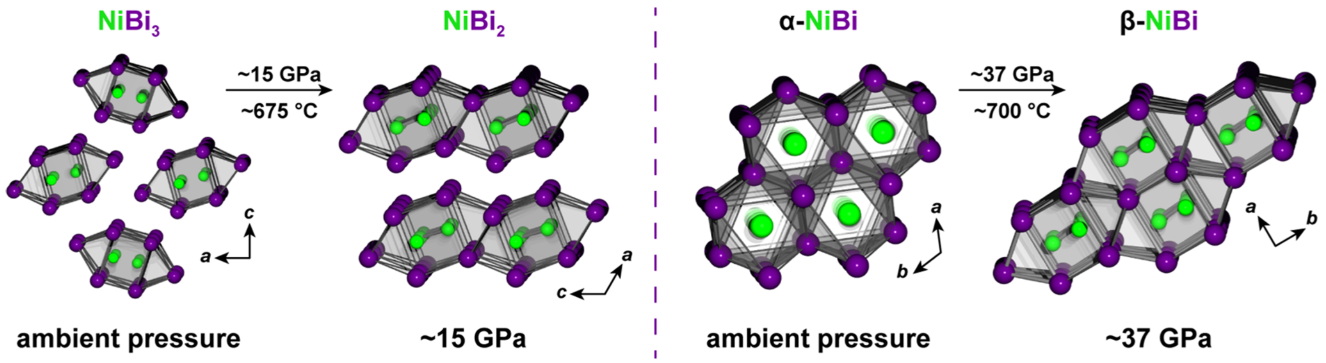

Figure 3. Polyhedral representation of the crystal structure of four known Ni−Bi intermetallic compounds. Violet and green spheres represent Bi and Ni, respectively. Thermodynamically stable precursor $NiBi_3$ forms layered $NiBi_2$ by heating at ∼15 GPa (left). Thermodynamically stable α-NiBi was previously reported to form β-NiBi upon heating at ∼37 GPa (right).[13] The polyhedral representation clearly depicts the identical subunits that form quasi-1D $NiBi_3$, quasi-2D $NiBi_2$, and compact β-NiBi.

Bi_7 monocapped trigonal prisms that are rectangle-face-sharing along the *b*-axis to form 1D $NiBi_3$ prism rods. In $NiBi_3$, these rods are spatially separated, connected by weak Bi−Bi bonds (Figure 3, left). In $NiBi_2$, the 1D prism rods are triangle-face-sharing perpendicular to their running direction, generating a layered structure. Strikingly, the structural motif of 1D rods is also present in the recently reported high-pressure β-NiBi phase (Figure 3, right).[13] In this structure, the 1D prism rods are triangle-face-sharing both perpendicular to their running direction and along the crystallographic *a*-axis, forming a compact three-dimensional (3D) structure. In elemental examples, it is common for atoms to increase coordination number and adopt close-packed arrangements under pressure.[20,23] This system is particularly interesting because as pressure is increased, the coordination of Ni remains constant such that the $NiBi_3$ prism rod motif is maintained. Instead, we observe an overall increase in dimensionality from the quasi-1D $NiBi_3$, to quasi-2D $NiBi_2$, to compact 3D β-NiBi by a "polymerization" of prism rod building blocks and a corresponding change in stoichiometry associated with a decrease in bismuth content. Note: β-NiBi has only been synthesized from α-NiBi, indicating that other factors also play an important role in going from one compound to another.

There is precedent for such behavior in the form of chemical pressure as a mechanism to control dimensionality. One example is within the AeNiGe (Ae = Mg, Ca, Sr, Ba) system, where an increase of the cation size led to a reduction of the dimensionality of the [NiGe] building blocks.[24] Further, the dimensionality of binary compounds comprised of light elements, such as SiS_2, can be controlled from 1D to 3D with relatively low physical pressure.[25] To the best of our knowledge, the Ni−Bi system is the only example of a binary intermetallic system where the structural subunits can pack from quasi-1D to quasi-2D and ultimately to 3D depending on the synthesis pressure and precursor stoichiometry. These results recommend the high-pressure exploration of other intermetallic systems that under ambient conditions exhibit low dimensionality, such as Ta_4SiTe_4,[26] $ZrTe_5$,[27] and $CoSn_3$.[28]

Although the new $NiBi_2$ phase forms from $NiBi_3$ with the expulsion of Bi at ∼14 GPa and ∼675 °C, previous experiments using α-NiBi as the precursor do not produce $NiBi_2$ at similar pressures and temperatures. When qualitatively determining which materials may be more stable at high pressure, the unit cell volume of the materials may be considered, as increasing pressure tends to favor higher densities in materials. Under temperature and pressure conditions at which $NiBi_2$ and Bi(V) form from $NiBi_3$, $NiBi_3$ has a unit cell volume of 85.6(1) $Å^3$ per formula unit, whereas $NiBi_2$ and Bi(V) have a combined unit cell volume per formula unit of 84.54(1) $Å^3$. Therefore, the formation of $NiBi_2$ is favorable from a density perspective, as the volume of the system decreases by 1.2% upon conversion from $NiBi_3$ to $NiBi_2$ + Bi(V). In comparison, at about 14.1(1) GPa, α-NiBi has a unit cell volume of 68.48(1) $Å^3$ per two formula units, whereas $NiBi_2$ + Ni have a combined volume of 70.50(8) $Å^3$ per formula unit.[29] Thus, forming $NiBi_2$ and Ni from α-NiBi requires a ∼3% increase in the summed volume of the phases, which is unfavorable from a density standpoint. This may account for why $NiBi_2$ forms from $NiBi_3$ but not from α-NiBi in this pressure range and reinforces the importance of stoichiometry in determining which products are formed at high-PT conditions.

After isolating the new phase at high-pressure conditions within the LH-DAC, we performed a decompression study to assess if the compound remained stable to ambient pressure, i.e., to determine whether it was pressure-quenchable (Figure S4). Bragg peaks corresponding to $NiBi_2$ persisted upon decompression to ambient pressure, indicating that the phase was in fact pressure-quenchable. We scaled-up the reaction using a multianvil press (MAP) to probe the physical properties of $NiBi_2$. The new binary compound was obtained in ∼75% yield by reaction of the elements at ∼15 GPa and ∼675 °C for 1 h (see Supporting Information for details). Scanning electron microscopy and energy dispersive X-ray spectroscopy performed on the decompressed sample confirmed that the majority of the sample consisted of $NiBi_2$ and indicated the presence of unreacted elements Ni and Bi as well as regions of Ni/Bi 1:1 and 2:1 (Figure S6). Because of the layered structure and the high-pressure synthesis conditions, crystals sufficiently large for single-crystal X-ray diffraction could not be isolated from the reaction product. The structure of $NiBi_2$ at ambient pressure was confirmed by the Rietveld refinement of the synchrotron PXRD pattern (Figure S9). A comparison of the high-pressure and ambient-pressure structures highlights the layered nature of the structure. The unit cell volume of the new phase increases by 16.3% upon decompression. Notably, the interlayer spacing increases by 16.8% upon decompression, indicating that the interlayer region, likely occupied by the Bi lone pair, is the area of highest compressibility in the structure (Figure 4). The

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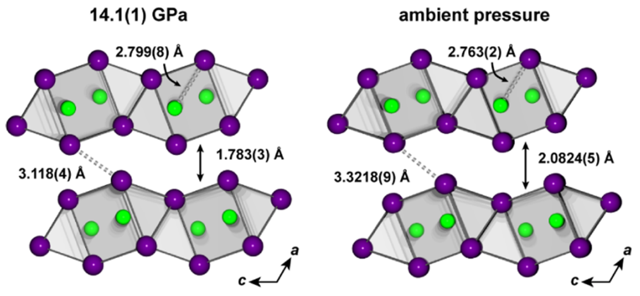

Figure 4. Comparison of the 14.1(1) GPa and ambient-pressure crystal structures of $NiBi_2$. Notably, the interlayer spacing increases by ~16% and the Ni1−Bi1 bond decreases by ~1.3%. Violet and green spheres represent Bi and Ni, respectively.

anisotropic compressibility of the sample is further emphasized by the surprising 1.3% decrease in the Ni1−Bi1 distance compared to the 6.5% increase in the Bi1−Bi1 interaction distance (Figure 4). The ambient-pressure Bi1−Bi1 distance (3.3218(9) Å) is slightly greater than twice the atomic radius of bismuth ($2r_a$ = 3.2 Å),[30] suggesting the possibility for a Bi−Bi bonding interaction between layers. Electronic structure calculations and detailed bonding analyses are necessary to evaluate the nature of this Bi−Bi interaction. The overall change in atomic distances from high pressure to ambient pressure, and the persistence of the network of strong Ni−Bi interactions, verifies the layered nature of the structure.

To purify the sample for physical properties measurements, we ground the as-synthesized sample from the high-pressure MAP reaction and magnetically separated the ferromagnetic elemental Ni component. Synchrotron PXRD indicates that unreacted elemental Ni is absent from the sample after magnetic separation and demonstrates that the sample consists of 74.4 wt % $NiBi_2$, 20.73 wt % Bi, and 4.8 wt % $NiBi_3$ (Figure S9). Preliminary variable-temperature dc magnetic susceptibility measurement of this sample acquired at H_{dc} = 5 Oe shows a broad and continuous downturn in susceptibility with an onset of T_c ~ 4.2 K (Figure S8). This behavior is indicative of a superconducting transition, however the broad nature of the transition, which is potentially due to strain in the 2D lattice or ferromagnetic amorphous Ni, prevents us from a definitive assignment of bulk superconductivity arising from this phase. It should be noted that the $NiBi_3$ impurity in the sample may be the source of the superconducting signal, as $NiBi_3$ is a superconductor. Our attribution of the superconductivity to a new phase arises largely from the higher T_c in the pellet described above (T_c ~ 4.2 for our sample; T_c = 4.06 for $NiBi_3$). This implies but does not confirm that superconductivity arises from a different phase than $NiBi_3$. Future measurements will focus on elucidating the physical properties of this material in higher purity samples and using additional techniques such as heat capacity and resistivity.

Calculations performed by Weihrich and co-workers in 2013, and in 2018 by Wolverton and co-workers, suggest that the monoclinic layered phase of $NiBi_2$ experimentally realized here should be stable with respect to decomposition at ambient pressure and should be synthetically accessible using traditional solid-state methods.[31,32] To assess the metastability of the high-pressure phase, we performed differential scanning calorimetry (Figure S7). Upon heating the sample, we observe an exothermic event at 262 °C immediately followed by the endothermic melting of elemental Bi at 271 °C. A corresponding crystallization event is not observed upon cooling, suggesting that $NiBi_2$ is in fact metastable. If the compound is metastable at ambient pressure, methods that promote atomic mixing at low or ambient temperature, such as molecular beam epitaxy or co-sputtering, may be able to successfully isolate this phase. This could further prove useful in generating thin-film samples for properties measurements. Importantly, it could have far-reaching implications for the low-temperature discovery of new phases in simple binary systems.

The foregoing results illustrate the high-PT synthesis of the new binary compound $NiBi_2$. This quasi-2D material exhibits the same basic structural unit present in the thermodynamically stable quasi-1D $NiBi_3$ and the metastable high-pressure phase β-NiBi. This structural continuity is suggestive of control of dimensionality via pressure and highlights the structural diversity that can be achieved at high pressures. Crucially, the newly isolated binary phase comprises a potentially exfoliable layered material bearing a heavy main-group element. Future studies will focus on increasing yield and exfoliating this material.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.chemmater.8b04412.

Schematic of DAC for in situ reactions, comparison of diffraction texture between phases at 14.1 GPa, coordination geometry of $NiBi_2$, PXRD patterns of the $NiBi_3$ decompression, schematic of modified 10/5 high-pressure cell assembly, scanning electron microscopy of $NiBi_2$, Rietveld refinement of PXRD of ambient-pressure $NiBi_2$, temperature-dependent molar direct current magnetic susceptibility, differential scanning calorimetry of $NiBi_2$, high-pressure and ambient-pressure refinement details for $NiBi_2$, list of atomic interactions for $NiBi_2$ (PDF)

High-pressure and ambient-pressure crystal structures (CIF) (CIF)

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Notes

The authors declare no competing financial interest.

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Chem. Mater. 2019, 31, 955−959