Microscopic Changes in $HoNi_2B_2C$ Due to Thermal Treatment, and Its Effect on Superconductivity

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The low-temperature properties of the quaternary borocarbide compound $HoNi_2B_2C$ (space group *I4/mmm*) strongly depend on its thermodynamic state established via thermal treatment with subsequent quenching. In order to resolve the microscopic origin of these changes, high resolution X-ray powder diffraction data were taken in flat plate geometry at ambient conditions with a wavelength of 0.7 Å at beamline X3B1 on a pair of polycrystalline sample halves with identical chemical composition ($HoNi_2B_{2.1}C$) but annealed at different temperatures, namely at 800ºC and at 1100ºC. Their superconducting transition temperatures differ by more than 10% (see Fig. 1).

Rietveld refinement of the two data sets in the range between 0.46 and 5.73 Å using the program system GSAS as well as an additional difference Fourier analysis reveal subtle differences in the atomic parameters and in the electron density on the carbon site (see Fig. 2 (d)) for the two different annealing temperatures. Furthermore, compared to an expected model plane, a new atomic site (Wyckoff position 8*g*) can be identified for both samples, which is partially occupied with the lighter atoms boron or carbon (see Fig. 2 (b) and (c)).

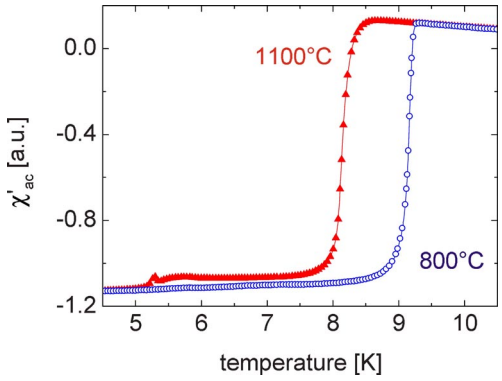

Figure 1. Low-temperature behavior of the real part of the ac susceptibility of two halves of a $HoNi_2B_{2.1}C$ sample, annealed at 800ºC (open circles) and at 1100ºC (filled triangles), showing clearly the strong dependence of the superconducting properties on the temperature of thermal equilibrium.

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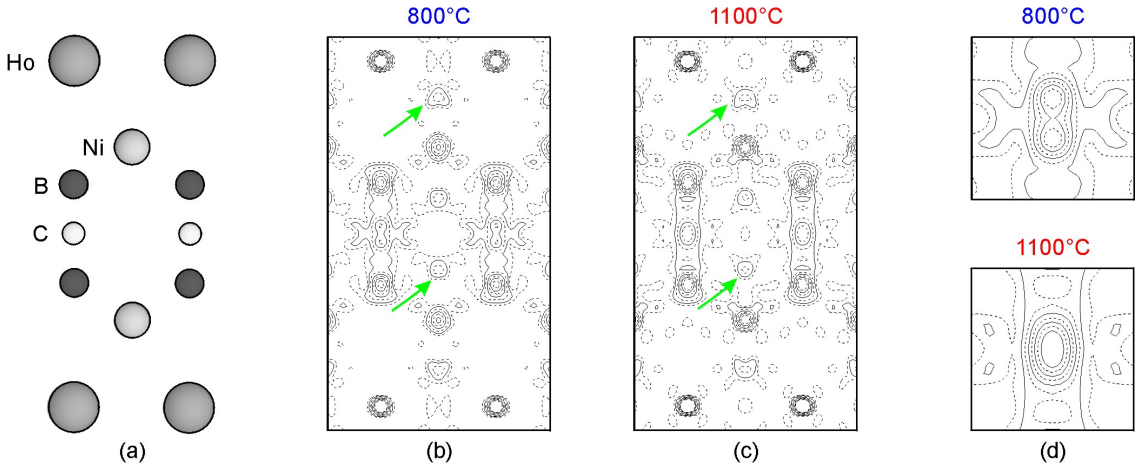

Figure 2. Difference Fourier maps of the (100) plane for the two $HoNi_2B_{2.1}C$ sample halves, annealed at 800ºC (b) and at 1100ºC (c) (map size: 7 × 12 $Å^2$). Contour lines are drawn for 0.5, 1.5, 3, 5, 7, 9, and 11 electrons per $Å^3$ with dotted and solid lines in alternating order. A sketch of the ideal structure is shown on the left hand side (a). Notice the "dog head-shaped" intensity marked with arrows in (b) and (c) (for the biologists among the readers: the position of the ears seems to be correlated with the annealing temperature). An enlargement of the carbon site (square area: 1 $Å^2$) is plotted in (d) with contour lines from 0.5 to 7.5 (the latter only for 1100ºC) in increments of one electron per $Å^3$.