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**Abstract:**

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"SDIO: Discovering Superconducting Materials at High Temperatures"

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Begin date: June 1, 1993
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Final Report

"Discovering Superconducting Materials at High Temperatures"

Professor Francis J. DiSalvo

The research funded under this grant focused on the layered structure compounds BaNiS$_2$ and BaCoS$_2$. The former is a metallic conductor while the latter is a magnetic Mott insulator. We planned doping studies to study the effects of both disorder and the crossover to the metallic state. It is hoped that doping a Mott insulator to the metallic state might produce a high temperature superconductor. Unfortunately, due to the termination of the SDIO program, this research was supported for only one year (instead of the planned three years), so the project is not complete.

We have shown that BaNiS$_2$ can be doped by copper to produce BaNi$_{1-x}$Cu$_x$S$_2$ for $x < 0.5$. It is rather surprising that this is possible, since in chalcogenides Cu is known to be +1 valence thus it formally requires the Ni to be +3. Of course, considerable covalency will mix the sulfur and nickel orbitals at the Fermi energy and ionic like oxidation states do not obtain. Upon doping with Cu, the metallic BaNiS$_2$ becomes less conducting with the room temperature resistance increasing by a factor of three and becoming almost temperature independent. It is likely that the large site disorder on the Ni lattice caused by Cu substitution is pushing the system towards Anderson localization. This work is almost complete and a publication is being readied.

The second phase of this project, doping BaCoS$_2$ with K to produce Ba$_{1-x}$K$_x$CoS$_2$, is only midstream. We are preforming K substitution in an attempt to dope this Mott insulator to the metallic state. In fact, while some K doping has occurred, the synthetic methods so far used all lead to some loss of K, which is quite volatile at the reaction temperatures (near 900 C). We are attempting to invent the proper synthetic technology to contain the K, but we are not assured success.

One publication has been accepted as a result of our years work: "Refined Structure and Properties of the Layered Mott Insulator BaCoS$_2" G. Jeffery Snyder, Maria C. Gelabert and F. J. DiSalvo, to be published in the Journal of Solid State Chemistry.

The graduate students supported in this project have been: Maria Gelabert, Sami Malik and Vincent Balberin.

There have been no patents or disclosures on this project.