ULTRANANOCRYSTALLINE DIAMOND FILMS AS ELECTRONIC MATERIALS.*

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The conversion of fullerenes as well as of hydrocarbons in hydrogen-poor argon microwave plasmas to phase-pure diamond results in a microstructure composed of 3-5 nm randomly-oriented crystallites. In such ultrananocrystalline diamond (UNCD) films, approximately 10% of the carbon atoms display considerable sp² bonding characteristics across two atom wide high energy, high angle twist grain boundaries (1,2). The addition of nitrogen to the synthesis gas gives highly electrically conducting films (up to 100 ohm cm⁻¹) with a slight temperature dependence indicating semimetallic behavior and activation energies in the meV range (3). Hall and Seebeck effect measurements prove that the conductivity is n-type in nature. Bulk carrier concentrations reach values of 10^{20} to 10^{21} cm⁻³, depending on plasma nitrogen content, with mobilities of 1-3 $/cm^2V^{-1}s^{-1}$ (4). Model quantum chemical calculations with nitrogen incorporated in the grain boundaries have given a detailed picture of the electronic energy level structure of n-type UNCD and are beginning to shed light on the conduction mechanism (5). UNCD films can also be doped p-type and both n and p-type UNCD films function extremely well as electrochemical electrodes (6,7).

In recent work, we have shown that a heterostructure consisting of UNCD grown on an epitaxial p-type single crystal layer of diamond shows 10-11 orders of magnitude of rectification with appreciable currents at ambient temperatures. Rectification occurs stably and reproducibly even at temperatures in excess of 1000 degrees Centigrade as might be expected for an all-carbon diode (8).

The fortuitous combination of excellent electrical conductivity coupled, because of the ultrananocrystallinity, with very low thermal conductivity (9) suggests the use of a combination of n and p-type UNCD as a new class of potentially high efficiency thermoelectric materials that can function at high temperatures as energy conversion devices. The ZT product is currently being studied as a function of temperature to evaluate figures of merit for these materials. *Work performed under the auspices of the US Department of Energy, BES-Materials Sciences, under Contract W-31-109-ENG-38

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