Materials Science & Engineering Thesis Defense

Theoretical investigation of transport across S/F interfaces

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abstract

The critical current density (Jc) is the most important device parameter for the Josephson junction devices used in the superconductor-ferromagnetic memory-circuits. In order to obtain sufficiently high Jc in the Josephson junctions, various combinations of superconductor (S) and ferromagnetic (F) materials are fabricated, then measured experimentally. This is an expensive and time consuming task. An improvement in the fundamental understanding of transport through the ferromagnetic layers and across the superconductor-ferromagnetic interface could potentially give fast, accurate predictions of the transport properties in devices and help guide the experimental studies. In this thesis, parameters calculated using density functional methods are used to model transport across Nb/Fe and Nb/Ni interfaces The model determines the transport parameters that arise when the following steps are used to simulate the transport: (a) transport through the superconductor with minimal loss in critical current, (b) conservation of crystal momentum (kll) and energy for one electron of the Cooper pair in the superconductor crossing the interface, followed by the second electron being transmitted within a coherence time and satisfying the Andreev reflection interfacial boundary conditions, (c) the influence of the field on the coherent pair in the bulk ferromagnetic and (d) spin-flip scattering in the bulk and at the interfaces. Our approach to model the interface transport focuses on determining the transport properties of the few select areas in k-space, often referred to as "hot spots", that satisfy conditions (b), (c) and (d). With iron, almost 75% of the current flows through one major "hot spot" and with nickel, more than 70% of the current flows through three major "hot spots". For accessing the transport of the correlated carriers through the ferromagnetic layer resulting from the proximity effect, the energy splitting between the minority and majority band at the respective points in k-space differ markedly from the analogous mean-field parameter, the exchange energy, assumed by earlier workers. We also include the pair-breaking mechanism of spin flip scattering at the interface and in the ferromagnetic bulk in the model so that we can quantify the reduction in the critical current from this mechanism. To summarize the approach of our model, we can determine the reduction in critical current at each "hot spot" based on its own set of electronic properties including, for example, the charge density, conductivity, bulk transmittivity and energy splitting between the minority and majority bands. It also shows that earlier assumptions that used the mean-field exchange energy to predict the order parameter's decay and rotation in the superconductor does not result in accurate predictions.

November 2, 2018; 10:30 AM; DISC 246