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Effect of dopants in Cu single grain boundaries[1] MATHIEU CESAR, McGill Univ, DANIEL GALL, Rensselaer Polytechnic Institute, HONG GUO, McGill Univ — The downscaling of integrated circuits is presently limited by the so called size effect in Cu interconnects. One of the two major contributions to this increased resistivity is known to be grain boundary (GB) electron scattering [1]. We demonstrated that Cu single GB resistance can be calculated accurately from first principles using a combination of plane wave density functional theory for structural relaxation and non-equilibrium Green's function for transport [2]. We now determine the effect of the presence of dopants in the GBs using the novel non-equilibrium coherent potential approximation [3] and discuss the possibility of reduced resistance in doped Cu GBs. [1]: T.S. Kuan, C.K. Inoki, G.S. Oehrlein, K. Rose, Y.P. Zhao, G.C. Wang, S.M. Rossnagel, and C. Cabral, MRS Proc. 612, D7.1.1 (2000). [2]: M. Cesar, D. Liu, D. Gall, and H. Guo, Phys. Rev. Appl. 2 (4), 044007 (2014). [3]: Y. Zhu, L. Liu, and H. Guo, Phys. Rev. B 88 (20), 205415 (2013).

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