Diversity of surface conduction in pyrite FeS$_2$ single crystals

CHRIS LEIGHTON, JEFF WALTER, XIN ZHANG, FRAZIER MORK, RYAN HOOL, MIKE MANNO, ERAY AYDIL, University of Minnesota — Pyrite FeS$_2$ has long been recognized as an attractive material for solar cells because of its high absorptivity, potential low cost, high abundance, and low toxicity. Despite having appropriate band gap (0.95 eV) and minority carrier diffusion length (100-1000 nm), low open circuit voltages ($V_{oc} \leq 0.1$ V) have plagued FeS$_2$-based cells. Surface conduction has been proposed as a contributing factor for the low $V_{oc}$, particularly a $p$-type surface inversion layer on $n$-type crystals [1]. Here we report a detailed electronic transport study of a large number of well-characterized CVT-grown $n$-FeS$_2$ single crystals. Abundant evidence of surface conduction is found from the $T$ dependence of resistivity, resistance anisotropy, low $T$ behavior at the 2D quantum resistance, thickness dependence, and the influence of contact metal work function. However, striking diversity in this surface conduction is found, even in nominally identical crystals at similar doping. The results cannot be understood by surface inversion alone, pointing to as yet uncontrolled surface factors. [1] Limpinsel et al. Energy Environ. Sci. (2014). Work supported by NSF.