Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Field-Emission from Chemically Functionalized Diamond Surfaces: Does Electron Affinity Picture Work? YOSHIYUKI MIYAMOTO, TAKEHIDE MIYAZAKI, DAISUKE TAKEUCHI, HIDEYO OKUSHI, SATOSHI YAMASAKI, AIST — By means of the time-dependent density functional electron dynamics, we have revisited the field-emission efficiency of chemically functionalized diamond (100) surfaces. In order to achieve high efficiency and high (chemical) stability, proper chemical species are needed to terminate diamond surfaces. Hydrogen (H) termination is well known to achieve the negative electron affinity (NEA) of diamond surface which indeed enhances field emission performance than that of clean surface with positive electron affinity (PEA). Yet, the durability of H-terminated diamond surface was concerned for long-time operation of the field-emission. Meantime, oxidation, or hydroxyl (OH) termination was considered to achieve chemical stability of the surface but presence of oxygen (O) atom should reduce the emission efficiency. Recently, H- OH-co-terminated surface is reported as NEA and was expected to achieve both emission efficiency and chemical stability. However, our simulation showed that emission efficiency of the H- OH- co-terminated surface is much lower than clean surface with PEA, thus we note that the electron affinity cannot be a unique measure to determine the emission efficiency. In this talk, we introduce necessity of new concept to understand the emission efficiency which needs to know detailed potential profile from bulk to vacuum through surface, which is strongly dependent on the surface chemical functionalization. This work was supported by ALCA project conducted by Japan Science and Technology Agency.

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Date submitted: 11 Nov 2013 Electronic form version 1.4