Abstract

First principles calculation reveals that the compressed (tensile) strain increases (decreases) the work function of Nb and W (110) surfaces, and that the interface dipole is formed in the Nb-W interface due to an unequal loss of the electrons from Nb and W interface atoms, and that the formation of the Nb-W interface is energetically favorable with negative interface energy, implying a tendency of interface interdiffusion of Nb and W atoms. Interestingly, the work function of Nb-W phases is insensitive to the composition as well as the Nb surface segregation when W is in the range of 0–60 at. %, and over this composition range the work function remains relatively stable.

Introduction

Importance of Metal Gate

Requirement of further miniaturization: 70 nm in 2006→45 nm in 2010→14 nm in 2020

Problem of polysilicon gate: polysilicon depletion; dopant penetration; gate leakage

Solution: metal gate!! Which metal?? far from decided yet!!

Work function and electronic structure of metal gate Nb-W system

First principles calculation reveals that the compressed (tensile) strain increases (decreases) the work function of Nb and W (110) surfaces, and that the interface dipole is formed in the Nb-W interface due to an unequal loss of the electrons from Nb and W interface atoms, and that the formation of the Nb-W interface is energetically favorable with negative interface energy, implying a tendency of interface interdiffusion of Nb and W atoms. Interestingly, the work function of Nb-W phases is insensitive to the composition as well as the Nb surface segregation when W is in the range of 0–60 at. %, and over this composition range the work function remains relatively stable.

Motivation

First principles calculation based on DFT and LDA is used to understand the effects of strain, interface, and composition on work function and electronic structure of Nb-W system

Effects of Strain on Work Function

In the strain range of -0.05 to 0.05, the WF change: Nb: -0.22 to 0.08 eV W: -0.20 to 0.31 eV

Surface dipole effect increases (decreases) with increase of compression (expansion);
Electronic structure effect decreases (increases) with increase of compression expansion

DOS of Bulk NbW at E_f

Composition has a nonlinear effect on the DOS at E_f
DOS at E_f has a minimum at the composition of 75 at. % W.

Effects of Composition on Work Function

17 compositions: W (0–16)
At each composition, all possible atomic configurations of Nb and W atoms are calculated, respectively
Optimized atomic structure at each composition: the atomic configuration with the lowest total energy

References

1. The International Technology Roadmap for Semiconductors. Available from: