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Experimental and theoretical research on heat cleaning process of GaAlAs photocathodes

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ABSTRACT

During the heat cleaning process of GaAlAs photocathodes, Ga_2O_3 and Al_2O_3 occur through chemical reaction. Adsorption models with Ga_2O_3 and Al_2O_3 on $Ga_{0.5}Al_{0.5}As(001)\beta_2\ (2\times4)$ phase are built and calculated through first-principles method. A heat cleaning experiment is performed. Combining the experimental and calculation results, heating temperature and chemical reactions at the surface are analyzed. Work function, electron transfer and dipole moment are analyzed, the reason why quantum efficiency of GaAlAs photocathodes are much lower than that of GaAs photocathodes is analyzed. Additionally, band structure and DOS curves are compared.

1. Introduction

The ocean contains rich underdeveloped resource such as: animals, shellfish, seaweed, petroleum, power and mineral, therefore marine detection becomes very important. With high quantum efficiency, low energy spread and high spin polarization, NEA GaAs photocathodes have been widely used in night vision image intensifiers [1–4], however, with strong noise and unavailability to be used around the clock, it is unsuitable for ocean detection. With property response wavelength, NEA GaAlAs photocathodes have an important application prospect for ocean exploration, marine communication and seabed imaging [5]. Additionally, GaAlAs can also be applied to the electron accelerators due to their good photoemission and long lifetime [6,7].

NEA GaAlAs photocathodes are prepared on GaAlAs surface in ultra-high vacuum(UHV) system (at least 10^{-8} Pa) [8,9] by cesium oxygen activation. Cesium oxygen activation should be processed on an atomically clean surface, during the growth and transport process, contamination (such as: oil, oxides and impurities) occurs at GaAlAs substrate, as a result, clean process should be processed on CaAlAs substrate before cesium oxygen activation. The surface clean process contain two steps: chemical cleaning and high-temperature purification. Chemical cleaning, processed outside UHV system, is purposed to removing oil, impurities and defects caused by polishing. Cleaning processed inside UHV system is mainly used to remove Oxides and Carbide and the main methods contains argon ion bombardment, heat cleaning and hydrogen atom purification technique [10–14]. The surface damage during argon ion bombardment is obviously exist, hydrogen atom purification technique is mainly used in the research of polarized electron source, heat cleaning is most commonly and most widely studied. The heat cleaning temperature of GaAs and GaAlAs is 650 °C and 700 °C respectively and the quantum efficiency of GaAlAs photocathode is substantially lower than GaAs photocathode. Theoretical research on mechanism of this phenomenon is scanty.

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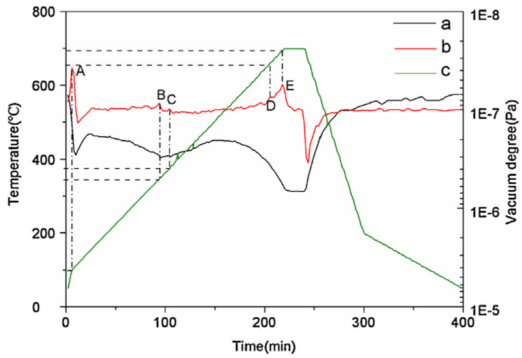

Fig. 1. Temperature (a), vacuum (b) and vacuum differential (c) curves during the heat cleaning process, P1–P5 show the peaks of vacuum differential curves.

In the present paper, a heat cleaning experiment is performed on GaAlAs substrate, adsorption models with Ga_2O_3 and Al_2O_3 on $Ga_{0.5}Al_{0.5}As(001)\beta_2$ (2×4) phase are built. Combining with first-principles [15,16] calculation method, the heating temperature is analyzed, chemical reactions during heat cleaning are analyzed. The reason of quantum efficiency of GaAlAs photocathode is substantially lower than GaAs photocathode is analyzed.

2. Method and calculation models

2.1. Heating cleaning experiment

An heat cleaning experiment was performed on GaAlAs substrate grown by metal organic chemical vapor deposition (MOCVD). The as grown sample was cut into some 10×10 mm samples. After chemical cleaning, the GaAlAs substrate was pushed into the pre-vacuum chamber. When the base pressure of UHV chamber is less than 3.3×10^{-8}Pa, the substrate was moved into the activation chamber and was put on the heating platform, at this moment, the vacuum went down, when the vacuum was stable, the heat cleaning experiment started. The steps is shown as curve(a) in the Fig. 1: the temperature increased from room temperature to 100 °C during 0–5 min, went on increases to 700 °C during 5–220 min, kept 700 °C during 220–250 min, cooled down from 700 °C to 200 °C during 250–300 min and then decreased to room temperature. The variation of vacuum, curve (b) in Fig. 1, is caused by the desorption of impurities at the surface. In order to analyze the desorption process, vacuum differential is added in Fig. 1 as curve (c). At certain moment of the heat cleaning process, As_2O_3 and GaAlAs will from Ga_2O_3, Al_2O_3 and As_2 through chemical reaction [2]. In consideration on this, Ga_2O_3 and Al_2O_3 adsorption $Ga_{0.5}Al_{0.5}As$ $(001)\beta_2$ (2×4) models are built and adsorption properties are compared.

2.2. Calculation method and models

The calculations is performed through the density functional theory (DFT) [16] by Cambridge Serial Total Energy Package (CASTEP). Generalized gradient approximation (GGA) [17] with the Perdew-Burke-Ernzerhof (PBE) functional is used. Atomic pseudopotentials is described through ultrasoft pseudopotential [18], the valence electrons contains Ga:$3d^{10}4s^24p^1$, Al:$3s^23p^1$, As:$4s^24p^3$, O:$2s^22p^4$ and H:1s. The energy cut off is set as 400 eV and the number of k points is set as $4 \times 6 \times 1$.

Fig. 2 depict Ga_2O_3 and Al_2O_3 adsorption $Ga_{0.5}Al_{0.5}As(001)\beta_2$ (2×4) models in our calculation. Al constituent is 0.5, the lattice parameter of $Ga_{0.5}Al_{0.5}As$ is 0.56572nm [19], β_2 (2×4) phase is chosen for GaAlAs surface [20]. Slab model is used in the calculation and the vacuum thickness of the slab models are 1.0nm [21].The reconstruction surface model is built with 7 layers of atoms [22]. During the optimization, atoms of top four layers are relaxed freely while the atoms of bottom three layers are fixed to simulate a bulk environment. A clean $GaAs(001)\beta_2$ (2×4) phase model with the same structure is built and the calculated work function is 4.764 eV, consistent well with the literature value 4.9eV [23], ensuring the reliability of our models.

3. Results and discussion

3.1. Adsorption energy and heating temperature

After adsorption, the position of atoms at $Ga_{0.5}Al_{0.5}As(001)\beta_2$ (2×4) surface is changed. The coordinate system in Fig. 2 is used to analyze the variation of Geometric structure. Formula (1) expresses the movement of certain atom. Comprehensive position variation of certain element can be calculated by formula (2).

$$\Delta l = \sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2} \quad (1)$$