第 22 卷第 7 期 半 导 体 学 报 Vol. 22, No. 7
2001 年 7 月 CHINESE JOURNAL OF SEMICONDUCTORS July, 2001

Modeling Thermodynamics of Smart-Cut Process*

HAN Wei-hua and YU Jin-zhong

(*State Key Laboratory on Integrated Optoelectronics, Institute of Semiconductors, The Chinese Academy of Sciences, Beijing* 100083, *China*)

Abstract: A thermodynamic model of hydrogen-induced silicon surface layer splitting with the help of an oxidized silicon wafer bonded is proposed. Wafer splitting is the result of lateral growth of hydrogen blisters in the entire implanted-hydrogen region during annealing. The blister growth rate depends on the effective activation energies of both hydrogen complex dissociation and hydrogen diffusion. The hydrogen blister radius was studied as the function of annealing time, annealing temperature and implantation dose. The critical radius was obtained according to the Griffith energy condition. The time required for wafer splitting at the cut temperature was calculated in accordance with the growth of hydrogen blisters.

Key words: thermodynamics; Smart-Cut process; splitting time; cut temperature
PACC: 6848; 6860; 7340T; 8265D
CLC number: TN301.1 **Document code**: A **Article ID**: 0253-4177(2001)07-0821-05

1 Introduction

There is a considerable interest in the process that a thin surface layer of a hydrogen-implanted silicon wafer is transferred onto an oxidized silicon wafer by bonding technology. With the help of the bonded wafer as a stiffener, a hydrogen-implanted wafer is split by the lateral growth of hydrogen blisters during annealing. This process has been commercially referred to as Smart-Cut process[1]. The advantages of this process are that implantation enables a high degree of uniformity of the top silicon layer to be obtained whereas the wafer bonding step keeps the good crystal quality of the silicon wafer to be preserved. Since the remaining wafer can be repolished and used again, Smart-Cut process has the potential to produce Silicon-On-Insulator wafers more economically than other competitive processes such as Separation by Implantation of Oxygen (SIMOX) and Bonding and Etch-back SOI (BESOI).

The thermal evolution of Smart-Cut process was studied in experiments as the function of implantation dose, annealing temperature and annealing time[2—4]. The growth of hydrogen blisters was found to be related intimately to the evaporation of trapped atomic hydrogens to molecular hydrogens in the blisters[5]. The time for large area layer splitting after bonding is about ten times longer than the time required to form hydrogen-induced surface blisters in unbonded samples. The effective activation energies of two procedures are basically same[6]. Neither microcavity formation nor silicon layer cleavage was observed at various annealing schemes between 200℃ and 900℃ outside the window of hydrogen implantation dose[7]. Freund[8] developed a model to estimate the lower bound of im-

* Project Supported by National Natural Science Foundation of China Under Grant Nos. 69990540 and 69896260-06 and "973" Plan Under Grant No. 20000366.

HAN Wei-hua male, born in 1973, doctor student. He is majoring in bonding materials on Si substrate.

Received 19 November 2000, revised manuscript received 30 March 2001

plantation dose for wafer splitting with the assumption of complete exfoliation. In this paper, we established the thermodynamic model of Smart-Cut process considering of the lateral growth of hydrogen blisters.

2 Criterion for Crack Growth in Bonded Hydrogen-Implanted Si Wafer

During implantation, the hydrogen ions collide with silicon atoms in the implanted region and interact with the existing defects (denoted as X), such as vacancies, interstitials and their agglomerates, to form hydrogen complexes X-H. During annealing, some trapped hydrogen atoms dissociate from X-H complexes and diffuse into the vacancies. Sufficient hydrogen pressure is exerted on the inner walls of blisters. With a bonded capping layer as stiffener, hydrogen blisters with radius a will anisotropically grow and overlap when the hydrogen pressure at the crack edges exceeds the fracture limit of silicon wafer. According to fracture mechanics, the opening displacement profile of the crack face in Fig. 1 is[8]

$$u_z(z = \pm 0, r) = \pm a \frac{p}{E} \times \frac{4(1 - v^2)}{\pi} \sqrt{1 - r^2/a^2} \tag{1}$$

where a is the radius of a hydrogen blister, p is the hydrogen pressure, E is Young's modulus, and ν is Poisson ratio. The volume of blisters expands with

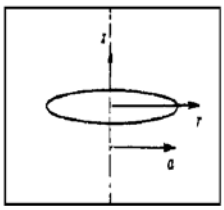

FIG. 1 Schematic Diagram of a Planar Crack with a Radius

the hydrogen agglomeration. Because of the evaporation of trapped atomic hydrogen, the inner gas pressure p remains to be a constant that is equivalent to the fracture limit of Si wafer. By integrating Eq. (1) over the crack area, the volume of the hydrogen blister is

$$\upsilon(a) = \frac{16}{3}(1 - \nu^2) a^3 p/E \tag{2}$$

The radius of a blister is determined by the strain energy U of bulk silicon around a blister, the crack surface energy Γ, and the external potential energy W. The elastic strain energy of bulk silicon around a blister is

$$U(a) = \frac{1}{2} \times \frac{E}{1 - \nu^2} \epsilon^2 \Omega, \tag{3}$$

where the strain $\epsilon = u_z(0)/a$, the strain volume $\Omega = 2\pi a^3$, Young's modulus is E, and Poisson ratio is ν. The crack surface energy of a blister is

$$\Gamma(a, T) = 2\gamma(T)\pi a^2, \tag{4}$$

where $\gamma(T)$ is the surface tension as the function of annealing temperature T. As the annealing temperature T increases, the evaporation of absorbed hydrogen on the passivated crack surface results in the said surface energy $\Gamma(a, T)$ being appreciably increased now. The external potential energy W is the hydrogen pressure acting through the crack face displacement, namely

$$W(a) = - p\upsilon(a) \tag{5}$$

Thus, the total free energy of a growing hydrogen blister is

$$G(a, T) = W(a) + U(a) + \Gamma(a, T) \tag{6}$$

According to the Griffith energy condition, the criterion for crack growth is taken to be

$$\frac{\partial G(a, T)}{\partial a} = 0 \tag{7}$$

Therefore, the critical radius for crack is

$$a_{crit} = \frac{\pi\gamma(T) E}{0.18 p^2 (1 - \nu^2)} \tag{8}$$

Figure 2 illustrates the total free energy $G(a)$ of a blister reaching its maximum at the critical radius a_{crit}. In the case of $a < a_{crit}$, since $\frac{dG(a)}{da} > 0$ holds, the blister is not stable and will shrink away. However, once $a \geqslant a_{crit}$, $G(a)$ will decrease with the increase of the blister radius a, and the blister can grow. If the radius a increases to a maximum value leading to $G(a) = 0$ before wafer splitting, the blister growth will end. Thus, the maximum radius

turns out to be

$$a_{max} = 1.5a_{crit} \tag{9}$$

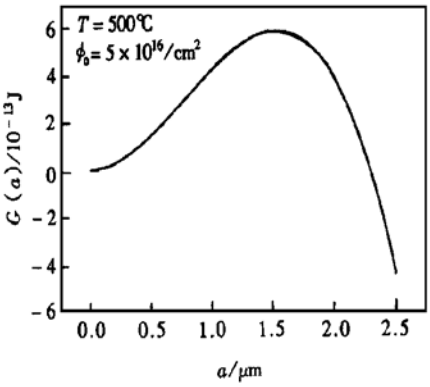

FIG. 2 Trend of Total Free Energy for a Growing Hydrogen Blister

3 Thermal Evolution of Hydrogen Blisters

The growth of hydrogen blisters is driven by the increased pressure of H_2. Trapped atomic hydrogen dissociates from hydrogen complex X—H with the activation energy E_a of 1.8eV, and diffuses with the energy E_d of 0.48eV into vacancies. Assuming that the hydrogen implantation dose is Φ_0 in silicon wafer before annealing, and the release hydrogen dose is Φ_e during annealing, then the rate of H_2 generation from the implanted region is

$$\frac{\partial\Phi_e(t,T)}{\partial t} = -k\Phi_e(t,T) \tag{10}$$

and the reaction rate constant is

$$k = \frac{1}{\tau}\exp\left(-\frac{E_a+E_d}{k_BT}\right) \tag{11}$$

where t is annealing time, T is annealing temperature, τ is phenomenological parameter, it is about 10^{-12} s, which relates to the stretching frequency of dissociating X—H bond, and k_B is the Boltzmann constant. All of the release hydrogen dose should be equal to the implantation dose Φ_0, namely

$$\Phi_0 = \int_0^\infty \Phi_e(t,T)\,dt \tag{12}$$

Therefore, the release hydrogen dose can be expressed as

$$\Phi_e(t,T) = k\Phi_0\exp(-kt) \tag{13}$$

The number N of the generated H_2 thus made available for pressurizing the opening crack should be

$$N = \pi a^2\int_0^t \Phi_e(t,T)\,dt \tag{14}$$

A hydrogen blister with the volume $v(a)$ and the gas pressure p will be fit to the ideal gas law

$$pv(a) = Nk_BT \tag{15}$$

If Eqs. (2) and (14) are substituted into Eq. (15), the blister radius a as a function of annealing temperature T, annealing time t and hydrogen implantation dose Φ_0 will be deduced as

$$a(t,T,\Phi_0) = \frac{3\pi E\Phi_0[1-\exp(-kt)]k_BT}{16(1-\nu^2)p^2} \tag{16}$$

When annealing time is long enough, namely $t=\infty$, there should exist a relation of

$$a(\infty,T,\Phi_0) = a_{max} \tag{17}$$

If we take typical parameters of $E = 1.66\times10^{11}$ N/m^2, $\nu = 0.29$, $p = 5\times10^8$ N/m^2, $\Phi_0 = 5\times10^{16}$/cm^2 in Eq. (17), the crack surface tension of a blister $\gamma(T)$ can be estimated to be about 0.1—0.2J/m^2 at temperatures of 450—700℃. Based on above parameters, typical curves of the blister radius for Eq. (16) are illustrated in Fig. 3, where the hydrogen blister radius increases very slowly at annealing temperature below 450℃. Figure 4 indicates that the radius of the hydrogen blister grows with annealing temperature, where the radius increases rapidly at the temperature of about 500℃ with the

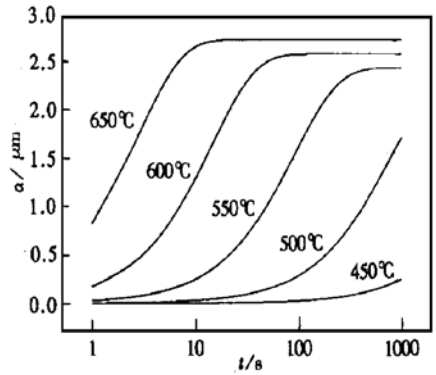

FIG. 3 Thermal Evolution of Hydrogen Blister as a Function of Annealing Time with Same Implantation Dose 5×10^{16}/cm^2 but at Different Annealing Temperatures

same annealing time 10^3s while for different implantation doses. The growth of hydrogen blister depends on the activation energy E_a and the diffusion energy E_d below about 540℃. As annealing temperature goes higher than about 540℃, the volume of hydrogen blister will expand with the increase of annealing temperature. It implies that all of implantation dose has been released before about 540℃.

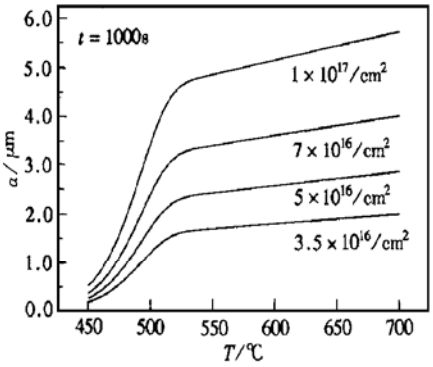

FIG. 4 Thermal Evolution of Hydrogen Blister as a Function of Annealing Temperature with Same Annealing Time 10^3s but for Different Implantation Doses

When implanted-hydrogen Si wafer begins to be splitting, the radius of the growing hydrogen blister should be equal to the critical radius for crack, namely

$$a(t, T, \Phi) = a_{crit} \tag{18}$$

Therefore, the splitting time as the function of the cut temperature is expressed as

$$t(T) = -10^{-12}\exp\left[\frac{E_a + E_d}{k_B T}\right]\ln\left[1 - \frac{14.8\gamma(T)}{k_B T \Phi_0}\right] \tag{19}$$

where crack surface tension may be phenomenologically expressed as $\gamma(T) = 1.5\times10^{-4}T + 5\times10^{-3}$J/m^2 according to Eq. (17). Figure 5 indicates the curves of splitting time as the function of annealing temperature for different implantation doses. The splitting time will become shorter at the fixed cut temperature with the increase of the hydrogen implantation dose.

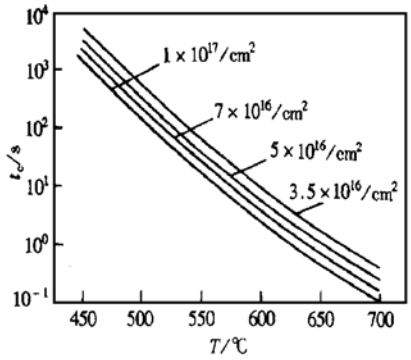

FIG. 5 Time Required to Wafer Splitting as a Function of Annealing Temperature for Different Implantation Doses

4 Conclusion

The study provides important process parameters concerning hydrogen-induced silicon surface layer cleavage. The hydrogen blister radius increases to a maximum value after enough annealing time. The hydrogen blister radius in hydrogen-implanted Si wafer increases rapidly at 500℃ for any fit implantation doses. The time for wafer splitting as the function of cut temperature mainly depends on both the activation energy and the hydrogen diffusion energy. The splitting time is shorter for the hydrogen-implanted Si wafer with a high implantation dose than for that with a low implantation dose.

References

[1] M. Bruel, Electron. Lett., 1995, **31**: 1201.

[2] M. K. Weldon, V. E. Marsico, Y. J. Chabal *et al.*, J. Vac. Sci. Technol., 1997, **B15**: 1065.

[3] B. Aspar, M. Bruel, H. Moriceau, C. Maleville *et al.*, Microelectron. Eng., 1997, **36**: 233.

[4] S. Y. Zhu, Y. P. Huang, A. Z. Li *et al.*, Chinese Journal of Semiconductors, 1999, **20**: 1071.

[5] C. M. Varma, Appl. Phys. Lett., 1997, **71**: 3519.

[6] Q.-Y. Tong, K. Gutjahr, S. Hopfe *et al.*, Appl. Phys. Lett., 1997, **70**: 1390.

[7] Xiang Lu, Nathan W. Cheung, Michael D. Strathman *et al.*, Appl. Phys. Lett., 1997, **71**: 1084.

[8] L. B. Freund, Appl. Phys. Lett., 1997, **70**: 3519.

智能剥离工艺的热动力学模型*

韩伟华　余金中

(中国科学院半导体研究所 集成光电子学国家重点联合实验室, 北京　100083)

摘要: 提出了注氢硅片表面借助键合氧化硅片进行剥离的热动力学模型, 这种剥离现象是退火过程中氢离子注入区氢气泡横向增长的结果. 氢气泡的增长速率依赖于氢复合体分解和氢分子扩散所需的激活能, 氢气泡的半径是退火时间、退火温度和注氢剂量的函数. 氢气泡的临界半径可根据 Griffith 能量平衡条件来获得. 根据氢气泡增长的这一临界条件, 获得了不同劈裂温度时所需的剥离时间.

关键词: 热动力学; 智能剥离; 剥离时间; 劈裂温度

PACC: 6848; 6860; 7340T; 8265D

中图分类号: TN301.1　　**文献标识码**: A　　**文章编号**: 0253-4177(2001)07-0821-05

* 国家自然科学基金(批准号: 69990540 和 69896260) 和国家"973"计划(批准号: 20000366) 资助项目.

韩伟华　男, 1973 年出生, 博士研究生, 目前主要从事硅衬底上键合材料的研究.

2000-11-19 收到, 2001-03-30 定稿