Thin films stress modeling : a novel approach

A.S.Bhattacharyya *, R.Praveen Kumar

Centre for Nanotechnology,
Central University of Jharkhand
Ranchi : 835205

*2006asb@gmail.com

A novel approach to estimate the thin film stress was discussed based on surface tension. The effect of temperature and film thickness was studies. The effect of stress on the film mechanical properties was observed.

Si-C-N thin films have been deposited by magnetron and its mechanical and structural characterizations have been done and published earlier [1-5]. The stress being developed in the films during deposition has major effects on the properties which have been dealt in this communication. The thickness of the film should increase with deposition time however an increase in thickness after a certain point may be detrimental for the mechanical properties of the films like hardness, modulus and adhesion.

The hardness and modulus increased substantially with deposition time and were maximum in the range of 60 to 80 minutes (Fig 1 a, b). The maximum hardness and modulus of 23GPa and 247GPa has been obtained for films deposited at 200 nm depth and deposited for 75 min (Fig 1c). For films deposited for higher deposition time the process of crystallization occurring in the films also attained stability. However on increasing the time further the thickness of the films increase as it being a function of deposition time. This enhanced thickness leads to larger residual stresses occurring in the films, which results in instability in the crystalline nature leading to a drop in hardness and modulus. Signature of high stress in terms of delamination being developed on 10μm thick coating on glass substrate is shown in fig 2.

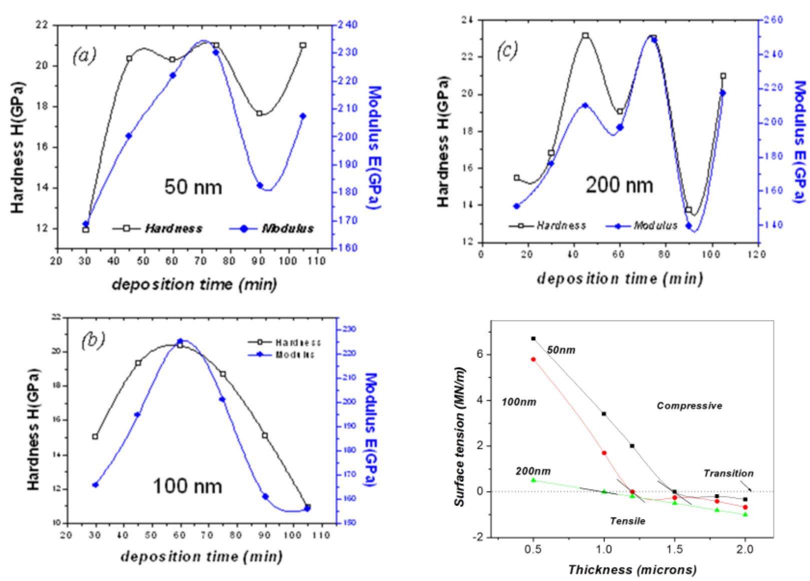

Fig 1: Hardness and modulus of SiCN films at different deposition times for nanoindentation penetration depth of (a) 50 nm (b) 100 nm and (c) 200nm. (d) Variation of surface tension with thickness.

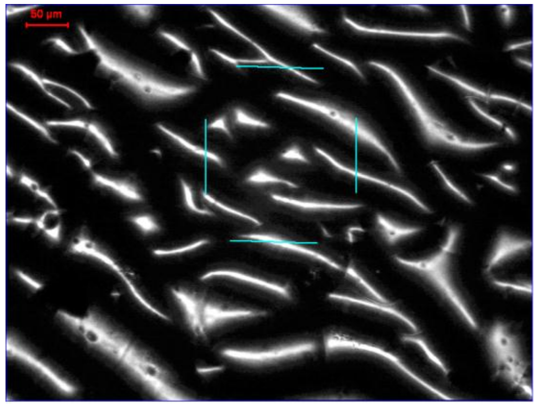

Fig 2: 10µm thick Si-C-N coating on glass substrate

The residual stress developing in the film is thus found to be a function of the deposition time .In analogy to the case of liquids, where the surface tension (S) decreases with rise in temperature following the Guggenheim-Katayama expression [6]

$$S = A\left(1 - \frac{T}{T_c}\right)^n \quad (1)$$

where T is the absolute temperature, T_c is the critical temperature, n is a constant whose value lies around 1.21 and A is a constant, an empirical relation can also be formatted for thin films

$$\zeta = \frac{dP}{dh}\left(1 - \frac{t}{t_c}\right) \quad (2)$$

Where t is the film thickness, t_c is the critical film thickness where residual stress becomes dominant. The constant n is taken to be unit and *dP/dh* is the slope of the load-depth curve in nanoindentation and determined from a tangent drawn to the loading part of the curve. The critical thickness tc where the residual stress becomes dominant and there is a drop in the H and E values as shown in Fig 6 (a) is a function of the deposition time for a particular condition of plasma parameters which in this case is 500^{o}C substrate temperature, 360W power and 1Pa pressure. The surface tension is positive at thickness lower than tc where compressive stresses are dominant and becomes zero where the transition from compressive to tensile stress occurs is zero according to the above formula. At thickness higher than tc however the surface tension becomes negative due to tensile stress. The critical thickness was 1.5µm for 50nm depth, 1.2 µm for 100nm and 1 µm for 50nm which shows it to be also a function of the indentation depth and decreases wit increase in depth of penetration. Thus the effect of substrate increases on the residual stress being developed as we go close to the substrate. The variation of residual stress with critical thickness tc (1 - 5 µm; tc (i) ; i=1:10) for a set of increasing film thickness t (100 nm to 5 µm ; t(j) with j = 1: 50) is shown in fig 3.

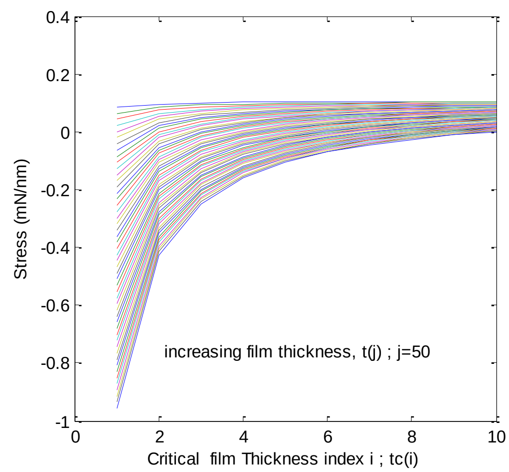

Fig 3: Residual stress at different critical thickness for increasing film thickness

A set of 27 experimental values of *dP/dh* were used for the simulation from an experimental nanoindentation load-depth curve. We obtained a (10 50 27) matrix of residual stress S (i, j, k). A stress which increases interatomic distance is tensile (positive) and which shortens it is compressive (negative). Work is done on each adatom coming to the surface against the action of an inward force before it attains a state of thermodynamic equilibrium. The residual stress arises therefore due to difference between the two.

A negative value of S is for tensile stress which is detrimental for the thin film whereas a positive value of S implying compressive stress is beneficial for the thin film. A zero value of S indicates no residual stress. From fig 3, it can be seen that the change in residual stress is much more turbulent in the lower thickness regime and we increase the film thickness, critical film thickness becomes gradually insignificant.

Reference

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