ANL/CP--76122

DE92 015227

Presented at the Spring 1992 meeting of the Materials Research Society, San Francisci CA, April 27-May 1, 1992

COMPUTER SIMULATION OF SCATTERED ION AND SPUTTERED SPECIES EFFECTS IN ION BEAM SPUTTER-DEPOSITION OF HIGH TEMPERATURE SUPERCONDUCTING THIN FILMS

ALAN R. KRAUSS* and ORLANDO AUCIELLO**

* Argonne National Laboratory, Chemistry and Materials Science Divisions, 9700 South Cass Ave., Argonne, IL 60439

** MCNC, Center for Microelectronics, 3021 Cornwallis Rd., Research Triangle Park, N.C. 27709-2889

ABSTRACT

Ion beam sputter-deposition is a technique currently used by many groups to produce single and multicomponent thin films. This technique provides several advantages over other deposition methods, which include the capability for yielding higher film density, accurate stoichiometry control, and smooth surfaces. However, the relatively high kinetic energies associated with ion beam sputtering also lead to difficulties if the process is not properly controlled. Computer simulations have been performed to determine net deposition rates, as well as the secondary erosion, lattice damage, and gas implantation in the films, associated with primary ions scattered from elemental Y, Ba and Cu targets used to produce high temperature superconducting Y-Ba-Cu-O films. The simulations were performed using the TRIM code for different ion masses and kinetic energies, and different deposition geometries. Results are presented for primary beams of Ar^+, Kr^+ and Xe^+ incident on Ba and Cu targets at 0° and 45° with respect to the surface normal, with the substrate positioned at 0° and 45°. The calculations indicate that the target composition, mass and kinetic energy of the primary beam, angle of incidence on the target, and position and orientation of the substrate affect the film damage and trapped primary beam gas by up to 5 orders of magnitude.

INTRODUCTION

Ion beam sputter-deposition is a technique with capabilities for producing complex multicomponent thin films and layered structures, in many cases with properties, over small and large areas, which are superior to those of films produced by other techniques. The method is well suited for in-situ synthesis of complex thin film structures. However, there are some aspects related to ion beam sputter-deposition which if not properly addressed can lead to undesirable effects that result in film property degradation. In many cases, the ions used to sputter the target material can be scattered towards the substrate with relatively high kinetic energies. This effect is especially pronounced when low mass ions such as Ar impact on high mass targets such as Ba or Bi. These energetic scattered ions can produce erosion of, and gas incorporation and lattice damage in the films. In the case of multicomponent thin films such as high temperature superconductors, preferential sputtering of the film components can occur, resulting in significant stoichiometric changes. Except for the issue of altered stoichiometry, the gas incorporation and damage effects pertain primarily to as-deposited films, rather than films which are subjected to high temperature post-deposition processing. However, the greatest benefit to be obtained from ion beam sputter-deposition relates to its ability to yield tailored sharp interfaces between materials of virtually any composition, benefits which are largely lost if high temperature post-deposition annealing steps are incorporated into the processing sequence.

The submitted manuscript has been authored by a contractor of the U. S. Government under contract No. W-31-109-ENG-38. Accordingly, the U. S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U. S. Government purposes.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

For deposition of multi-component films, a single target similar in composition to the desired film is often used. In principle, once the target has been "conditioned" by prolonged sputtering, the composition of the film should be the same as the composition of the target [1]. In practice however, it often occurs that as a result of diffusion, evaporation and segregation phenomena in the target, and low sticking coefficients of depositing species at the substrate and high resputtering rates by backscattered primary ions, the composition of the film does not match that of the target [1]. The target composition must then be deliberately modified in order to produce films of a desired stoichiometry. Alternatively, multicomponent films can be produced by sequential sputtering of elemental targets with a single ion beam [1-3] or simultaneous sputtering of multiple elemental targets with multiple ion beams [4]. The films produced by the last two methods are also affected by scattered ions from the target. For all the techniques described above, the extent of modification observed in the film depends on the mass and kinetic energy of the ion species, deposition rate, and deposition geometry. Additionally, these parameters also influence the amount of film damage and the amount of beam gas which is implanted into the film. For a given target stoichiometry, the deposition conditions required to produce the correct film stoichiometry are not necessarily the conditions which result in the best film properties in terms of implanted beam gas and film damage. In general, the composition of films produced from such targets may be history-dependent, and in exceptional cases, it has been found [5] that there are conditions under which no amount of target compensa. . will produce a given film stoichiometry.

The control of film stoichiometry in ion beam sputter-deposition is particularly difficult when using high energy, low mass ion beams to produce films containing heavy elements with low surface binding energies, such as Pb in the ferroelectric material $PbZr_rTi_{1-x}O_3$ (PZT), and Ba and Bi in $YBa_2Cu_3O_{7-x}$ and the Bi-Sr-Ca-Cu-O family of high temperature superconductors respectively. These materials have very high sputtering yields because of their low surface binding energies, and high primary ion reflection coefficients because of their high mass. For example, a 1 keV Ar^+ ion beam incident on Ba is reflected with kinetic energies of up to 800 eV. Consequently, the erosion of a growing film, by reflected primary ions, can be substantial as demonstrated in recent experiments [6]. However, by modifying the geometry and using Kr^+ or Xe^+ ions, rather than Ar^+, it is possible to reduce the secondary sputtering effects and control the degree of gas implantation and the amount of energy deposited into the film. Uncontrolled bombardment of growing films by ions scattered from the target have also resulted in undesirable effects on other system materials such as Pt/Co multilayered structures [7].

It is sometimes desirable to minimize or eliminate the uncontrolled deposition of high kinetic energy into a film by ions scattered from a target. On the other hand, it has been demonstrated [8] that in some cases a controlled deposition of energy into a growing film by bombardment with low energy (30 to 100 eV) ions can be used to improve film properties. For films or bulk samples of randomly mixed $YBa_2Cu_3O_{7-x}$, an 850-900 °C annealing process is frequently used to form the perovskite crystal structure of the superconducting phase. This temperature, which is incompatible with the preservation of sharply defined interfaces between thin layers of different materials in thin films, may be reduced if the target atoms are deposited with a few ten's of eV of kinetic energy or if low energy (ten's of eV) ions are purposely but controllably directed at the growing film. In general, it is possible to take advantage of ion-surface interactions to enhance adatom surface migration, resulting in the production of a given phase at a lower temperature than that required at thermodynamic equilibrium [9]. Deposition of the as-deposited superconducting phase of $YBa_2Cu_3O_{7-x}$ has been reported for substrate temperatures as low as 500 °C by controlling the kinetic energy of the target atoms as they impinge on the substrate [10].

Experiments performed in our laboratory [6,11] have demonstrated that by using Kr^+ or Xe^+ ion beams rather than Ar^+ ions, and adjusting the beam energy and angle of incidence with respect to the target, it is possible to reduce, minimize, or eliminate deleterious effects such as erosion of, and gas incorporation and damage produced in high temperature superconducting films

due to ions scattered from the target. One of the undesirable effects of primary ion scattering recently observed in our laboratory [11] is particularly relevant to the discussion in this paper and relates to the fact that the T_c's of YBCO films, produced by sputtering of a stoichiometric YBCO target with a Xe^+ ion beam, increase from 70 K to 86 K as the energy of the Xe^+ beam decreases from 1200 to 500 eV. The implications of these results will be discussed later in this paper.

The discussion presented above indicates that it is important to understand the ion scattering and sputtering processes in ion beam sputter-deposition of multicomponent thin films in order to understand and control the synthesis-microstructure-property relationships of these films. Therefore, It is the purpose of this paper to quantitatively evaluate the role of geometric effects and the ion beam mass and kinetic energy as they pertain to multicomponent thin film deposition. $YBa_2Cu_3O_{7-x}$ will be used as the test material although the formalism is general enough that it can be applied to other materials. Specifically, an objective of this paper is to provide researchers with a tool that could be used to determine the best possible geometry and deposition conditions before attempting to produce single or multicomponent thin films by ion beam sputter-deposition.

COMPUTER SIMULATIONS OF ION SCATTERING AND SPUTTERING PROCESSES

In order to understand and control the processes involved in the synthesis of high temperature superconducting thin films by ion beam sputter-deposition, we have initiated a coordinated experimental and theoretical program to study ion scattering and sputtering processes involved in the deposition of these films. Since YBaCuO is one of the most widely investigated systems, the program has been focused on understanding the effects of primary ion beam backscattering on the production of $YBa_2Cu_3O_{7-x}$ thin films. The studies undertaken in the present work relate to the ion beam sputter-deposition technique developed by our group [2], where a single ion beam is used to sputter elemental target materials sequentially exposed under the beam to produce films with controlled stoichiometry. In this technique, the composition of the films is controlled by a quartz crystal resonator, appropriately positioned with respect to the substrate, which measures the thickness of each deposited elemental layer and sends a feedback signal to a computer to stop deposition as pre-programed layer thickness are reached [2]. However, the results obtained from the studies on sputtering and ion scattering phenomena discussed in this paper can be applied also to ion beam sputter-deposition techniques that involve the use of composite targets or multiple ion beams impacting on multiple elemental targets [4].

Three experimental geometries and deposition conditions have been chosen for the complete set of studies related to our research program, namely: (a) 0, 15, 30 and 45 degree angles of ion beam incidence with respect to the target normal (see Fig. 1), and (b) use of Ar^+, Kr^+ or Xe^+ ions with kinetic energies ranging from 500 eV to 5 keV. The experimental work includes analyses of scattered ions trapped in the films by secondary ion mass spectrometry (SIMS) and measurements of the film deposition rates for the different geometries indicated above. Preliminary experimental results related to this work have been reported elsewhere [6], and a more comprehensive experimental study is in progress. Therefore, this paper is focused on the computer simulations performed by using the TRIM code [12].

Calculations have been done for Ar^+, Kr^+ and Xe^+ ions with kinetic energies ranging from 50 to 5000 eV. The kinetic energy and angular distribution profiles of sputtered atoms and scattered primary ions from the target are used to provide an energy distribution function for the fluxes incident on the substrate. The results are used to predict the expected deposition and erosion rates, and scattered ion-induced gas implantation and damage in the films. The latter quantity is expressed in units of eV deposited into the film for each target atom deposited into the film, normalized to the number of primary ions incident on the target. The kinetic energy of each

scattered primary ion incident on the film is not however, uniformly distributed over the entire film. Instead, the energy is deposited into a very small volume associated with each collision cascade. The volume of the cascade is itself a function of the primary mass, kinetic energy and angle of incidence on the substrate, as well as the composition of the film. The kinetic energy imparted to a given film atom may therefore be much higher (typically 10's of eVs) than the values reported here. More complete results will be reported elsewhere [13]. However, the degree of atomic displacement damage is in general, proportional to the total deposited kinetic energy, and for the purpose of the present discussion, it is sufficient to ignore the spatial distribution of kinetic energy within the film.

The TRIM program [12] is a Monte Carlo code which calculates the development of the collision cascade generated by a fast particle impacting on a solid at an angle θ_i with respect to the surface normal. The interaction between colliding atoms in the solid is described by an empirical interatomic potential, and the atoms are considered to be randomly distributed, with a mean atomic spacing equal to the average lattice parameter. The primary ion trajectory and the trajectories of all particles within the collision cascade are followed by the program until the kinetic energy falls below a cut-off energy beyond which no further displacement of atoms from lattice positions or surface ejection events occur. TRIM is used to calculate the sputtered target atom and ion scattered primary ion flux distributions, which are subsequently used in the mathematical formulation presented in the next section to calculate film deposition and erosion rates, damage and beam gas implantation.

The surface binding energies of the target atoms are taken as the heat of sublimation (H_{Ba} = 1.91 eV, H_{Cu} = 3.5 eV, H_Y = 4.41 eV). Due to space limitations, the data presented in this paper relate only to 0° and 45° incidence of Ar^+, Kr^+, and Xe^+ ions onto Ba and Cu targets (The calculations indicate that the results for Y are not much different than for Cu), with substrate placement such that the scattered flux direction is at 0° or 45° with respect to the target normal (see Fig. 1). Two substrate orientations (θ_i') are considered, one in which the substrate is parallel to the target, and one in which the sputtered and ion scattered flux from the target is normally incident on the substrate. (see Fig. 1). A more complete report including all computer simulation results is in preparation [13].

GEOMETRY AND MATHEMATICS OF THE PROBLEM

TRIM calculations have been performed for 0° and 45° angles of incidence of the ion beam with respect to the surface normal of Y, Ba and Cu targets. The kinetic energies and polar (θ) and azimuthal (Φ) emission angles relative to the surface normal are calculated for all atoms which are sputtered from the target, and all primary ions which are scattered from the target surface. The kinetic energies of the scattered/sputtered particles are histogrammed into intervals equal to 1% of the primary ion kinetic energy, and the polar and azimuthal angular resolution is set at 3°. In order to obtain adequate statistics, the ratio of scattered primary ions/sputtered target atoms presented here represent an integration over the entire azimuth. However, both the scattered primaries and sputtered target atoms exhibit a peaking in the forward azimuthal direction (θ_o=θ_i, Φ=180^0, see Fig. 1). The approximation of using the complete azimuth rather than just a limited angular range somewhat underestimates the effect of scattered primary ions in the forward direction since the scattering exhibits a sharper forward peak than sputtering.

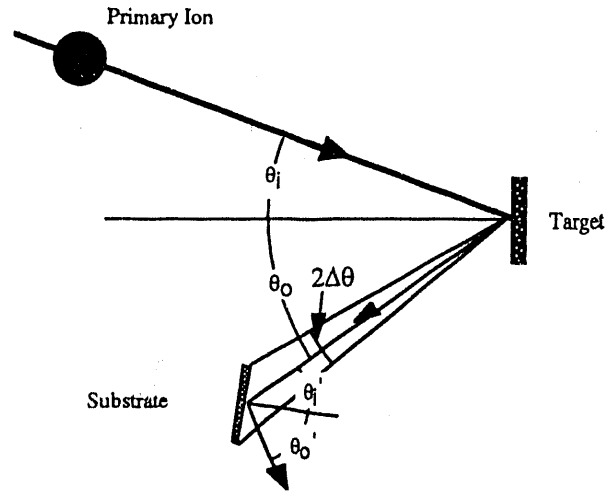

Figure 1. Geometry used for the computer simulations (see text for a description of angles).

Referring to Figure 1, a primary ion with mass M_1 and kinetic energy E_i is incident on the target at an angle θ_i, and the substrate lies in a direction θ_o in the plane of ion beam incidence, subtending an angle $\Delta\theta$. The substrate is tipped such that the sputtered target atoms and scattered primary ions are incident on the substrate at an angle θ_i'. Primary ions undergoing a second scattering from the substrate leave the surface at an angle θ_o'. All plots are labelled according to the angles of incidence of the primary beam on the target (θ_i), angle of substrate placement θ_o, and angle of scattered flux from the substrate θ_o' e.g. 45-0-45 indicates $\theta_i = 45^o$, $\theta_o = 0^o$, and $\theta_i' = 45^o$ (Fig. 1).

If a number, N_h, of primary ions are incident on the target, with kinetic energy E_i at an angle θ_i, then a number $S(E_i,\theta_i \mid E_o,\theta_o)$ of target atoms will be ejected at a polar angle between θ_o and $\theta_o+\Delta\theta$ with kinetic energy between E_o and $E_o+\Delta E$. All data presented were calculated for $N_h=10^4$ particle histories. The notation $S(E_j, \theta_j \mid E_k, \theta_k)$, $R(E_j, \theta_j \mid E_k, \theta_k)$ refers to the number of particles which are incident on a surface (target or substrate) with kinetic energy E_j, at an angle θ_j and sputtered (S) or reflected (R) into an angle θ_k with kinetic energy E_k. If the quantity S or R represents an integration over the "exit values", then the parameters to the right of the "|" symbol are omitted. The total number of sputtered target atoms $S(E_i,\theta_i \mid)$ may be found by summing over all angles θ_o and kinetic energies E_o. Since the substrate may be tilted relative to the line between the centers of the target and substrate, the target atom flux, defined as the number of target atoms deposited on the substrate per cm^2/incident primary ion on the target is given by:

$$\Phi\,(E_i,\theta_i,E_o,\theta_o,\theta'_i) = \frac{1}{N_h}\, S(E_i,\theta_i \mid E_o,\theta_o)\,\cos\theta'_i \tag{1}$$

where θ_i' is the angle between the substrate normal and the incident flux of sputtered target atoms. The deposition rate is determined by the number of target atoms which are deposited into the solid angle subtended by the substrate, taken here as the range between θ_o and $\theta_o+\Delta\theta$, integrated over the kinetic energy E_o.

$$\Omega = \sum_{E_o} \Phi\,(E_i\,,\theta_i,\,E_o,\,\theta_o,\,\theta_i') \tag{2}$$

In writing Eq. 2, we are implicitly assuming that since the kinetic energies of the sputtered atoms are at most a few tens of eVs, the sticking coefficient is nearly unity, regardless of the kinetic energy. This assumption is reasonable for substrates which are close to room temperature. For deposition of films at higher temperature ($\geq 500\ ^oC$), a present necessary condition to produce as-deposited high temperature superconducting thin films for example, a sticking coefficient smaller than one will be needed in the formulation. This will require the inclusion of a term that accounts for evaporation of deposited species, and will be part of future work.

The quantity $R(E_i,\theta_i \mid E_o,\theta_o)$ is defined as the number of primary ions which are scattered with kinetic energy between E_o and $E_o+\Delta E$ into a polar angle between θ_o and $\theta_o+\Delta\theta$ for N_h ions incident on the target at angle θ_i with kinetic energy E_i. This quantity directly affects film damage, gas implantation and resputtering effects. Both the absolute number of scattered ions and the kinetic energy distribution are strongly dependent on the angle of incidence and the mass of the primary ion. For e.g. Ar^+ ions impacting on Ba at 45°, we find that there are large numbers of scattered ions with kinetic energies > 400 eV, with a tail extending to 800 eV, i.e. 80% of the primary energy. On the other hand, for $N_h = 10^4$ Xe^+ ions normally incident on Cu, there was not a single ion scattering event predicted by TRIM. $R(E_i,\theta_i \mid E_o,\theta_o)$ represents a distribution function which provides the source term for the flux of energetic ions incident on the substrate. This distribution function is convoluted with the kinetic energy, sputtering yield and trapping efficiency to determine the lattice damage energy, secondary sputtering and implanted gas, respectively.

The flux of scattered primary ions to the substrate per incident primary ion at the target is given by :

$$\Phi^R\,(E_i,\theta_i,E_o,\theta_o,\theta'_i) = \frac{1}{N_h}\;R(E_i,\theta_i \mid E_o,\theta_o)\,\cos\theta'_i\,. \tag{3}$$

The quantity $\Phi^R\,(E_i,\theta_i,E_o,\theta_o,\theta_i')$ is peaked at low kinetic energies, with a tail extending to the value corresponding to a single collision between the primary ion and a surface atom. The present version of TRIM, however, specifically excludes single scattering events and therefore underestimates the extent of the high energy scattered primary ions. For oblique incidence , there is a tendency for both the scattered and sputtered fluxes to peak in the forward direction. However, the scattered primary ion flux is more peaked in the forward direction than the sputtered atom flux, and a substrate placed in the forward scattering direction will experience a higher energy flux of scattered primary ions than predicted for the azimuthally averaged flux. As a consequence of the lack of representation of single-collision events and the azimuthal averaging, the relative importance of primary ion scattering is underestimated. This omission will be corrected in future calculations [13].

Film damage, as measured by the kinetic energy deposited into the film by primary ions which are scattered from the target to the substrate, per primary ion incident on the target, is given by

$$\delta = \sum_{E_i} E_i'\,\Phi^R\,(E_i,\theta_i,E_o,\theta_o,\theta_i') \tag{4}$$

It should be noted that δ represents the total amount of kinetic energy which is deposited in the

film by ions scattered from the target, regardless of the kinetic energy distribution of the flux impacting on the growing film and the lattice displacement energy of the film atoms. Consequently, the quantity referred to here as "damage" is related to the actual damage, i.e., displacement of atoms from the lattice positions with the creation of vacancies and interstitials, but does not account for differences in lattice displacement energies between different film constituents. Additionally, as discussed earlier, the calculated quantity δ does not take into account the actual volume of the collision cascade into which the energy is deposited.

The secondary erosion associated with sputtering by scattered primary ions incident on the growing film is given by:

$$\varepsilon = \frac{1}{N_s} \sum_{E_i'} S(E_i', \theta_i' \mid) \quad \Phi^R (E_i, \theta_i, E_o, \theta_o, \theta_i') \tag{5}$$

The quantity $S(E_i', \theta_i' \mid)$ is the number of atoms sputtered from the film by N_s (scattered) primary ions incident at an angle θ_i', energy E_i' as defined earlier for the target with primary ions incident at an angle θ_o and energy E_o. The value of ε for ions with arbitrary kinetic energy E_i' incident on the substrate at an angle θ_i' is interpolated from the total sputtering yields (i.e. integrated over all exit angles and energies) calculated by TRIM for incident ion energies ranging from 50 to 5000 eV.

The net growth rate, defined as the number of target atoms/cm^2 remaining on the substrate per primary ion incident on the target is given by:

$$G = \Omega - \varepsilon. \tag{6}$$

In order to calculate the rate at which primary ions are implanted into the film, we need merely to integrate the scattered ion flux into the solid angle represented by the polar angle range θ_o to $\theta_o + \Delta\theta$ over the energy range from 0 to E_i.

$$GI = \frac{1}{N_h} \sum_{E_o = E_i'} R(E_i, \theta_i \mid E_o, \theta_o) \cos(\theta_i') \frac{1 - R(E_i', \theta_i' \mid)}{N_h} \tag{7}$$

Since some of the film will be eroded by secondary sputtering, a proportional amount of the implanted gas is also lost. The amount of gas retained in the film is therefore given by:

$$GR = GI\,(1 - \varepsilon/\Omega). \tag{8}$$

RESULTS AND DISCUSSION

Due to space limitations, only the calculations for Ar^+, Kr^+, and Xe^+ ions impacting on Ba and Cu targets at 0° and 45° angle of incidence with respect to the surface normal are discussed in this paper. The cases for these two angles of incidence have been selected because they represent a favorable and an unfavorable case, respectively, in terms of the effect of scattered ions on the film growth and properties. Because of space constraints, only calculations of damage and gas trapping in the films, are presented in this paper. The complete series of calculations including growth and erosion rates of the films will be presented elsewhere.[13] However, it is relevant to point out that

the limited experimental evidence on the effect of scattered ions on YBCO film properties obtained in our laboratory [11], together with the calculations presented here, indicate that ion-induced damage may be the dominant mechanism affecting film properties.

Normalized curves of damage/growth and trapped gas are presented in Figs. 2 and 3 for the primary ion/target combinations mentioned above. As discussed previously, the damage values are to be considered qualitative, both because the kinetic energy distribution and the degree of spatial localization are unspecified. The values for the trapped gas however, are absolute atomic concentrations in the film.

In general, it is found that the film damage increases with increasing primary ion energy, while the trapped gas decreases with increasing primary ion energy. Bombardment of the growing film by scattered Ar^+ ions results in the largest damage and trapped gas, while bombardment by Xe^+ results in the least. Regardless of the primary ion mass, 45° incidence of the primary beam on the target results in significantly more damage and gas implantation than normal incidence, in spite of the higher deposition rate associated with off-normal incidence. Finally, the low surface binding energy of Ba and high reflection coefficient, especially for relatively low mass primary ions such as Ar^+, makes Ba much more susceptible to beam damage and gas implantation than Cu or Y.

A comparison of Figs. 2a and 2b indicates that for a normally incident ion beam, the damage produced in the growing film by Ar^+ ions scattered from a Ba target is about an order of magnitude larger than the damage produced by Ar^+ ions scattered from a Cu target. For Kr^+ ions incident on Ba, the damage is approximately one order of magnitude lower than for Ar^+ incident on Ba, while the damage associated with Xe^+ incident on Ba is an additional factor of ten lower. For the Kr^+ and Xe^+ beams incident on a Cu target, the indicated damage/growth ratio is 3-4 orders of magnitude lower for the Ar^+ beam incident on Cu. The apparent equivalence between Kr^+ and Xe^+ is actually a result of the very low numbers of scattering events predicted by TRIM for these particle-target material combinations, and is to be taken as an upper limit for the actual damage/growth ratio.

The amount of gas trapped in the film decreases with increasing energy for all three primary ions scattered from Ba and for the Ar^+ ions reflected from Cu. However, for the latter target material, not a single scattering event in 10^4 particle histories was predicted for either Kr^+ or Xe^+, and it is concluded that for normal incidence virtually no Kr^+ or Xe^+ will be trapped in the film. Two relevant features of Fig. 2a should be pointed out; that is, the damage produced by scattered Xe^+ ions decreases noticeably when the energy of the primary beam impacting on the target is reduced from 1000 eV to 500 eV, while the amount of trapped gas increases. We have produced as-deposited superconducting $YBa_2Cu_3O_{7-x}$ films by ion beam deposition, using a range of primary energies, and find [11] that for a Xe^+ ion beam, the value of T_c decreases reproducibly from 86 K to 70 K as the kinetic energy increases from 500 eV to 1200 eV. For an Ar+ ion beam, the T_c values are even lower, assuming that the film is superconducting at all. This indicates that damage produced in the growing film by the scattered ions, rather than trapped beam gas, may be the dominant degradation mechanism.

Finally, the calculations of damage and amount of trapped gas in the growing film for all ions impacting on Ba and Cu at 45° (θ_i = 45° and θ_o = 45°) are presented in Figs 3a and 3b, respectively. The general trends of all curves presented in Figs. 3a and 3b as a function of the primary ion beam energy are similar to those discussed above for the case of normal incidence. However, there are four distinctive differences, namely: (a) the damage produced by Xe^+ ions scattered from Ba and Cu, for a 45° primary ion incidence, are about one and three orders of

magnitude larger, respectively, than the damage produced for normal incidence (Figs. 2a and 2b); (b) the difference in the film damage for the three ion species is not as large as it is in the normal incidence case (see Figs. 2a and 2b); (c) there is a noticeable difference in the damage produced by Kr^{+} ions with respect to that produced by Xe^{+} when scattered from Cu (Fig. 3b); (d) the amount of trapped gas is consistently higher than for normal incidence. Specifically, there is no target material, primary ion mass or kinetic energy for which no scattering events are observed.

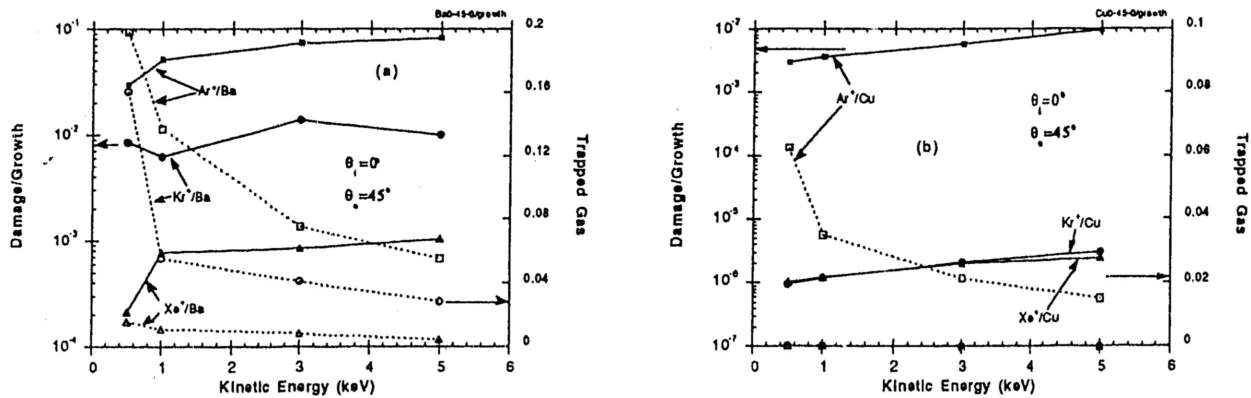

Figure 2. Normalized damage/growth and trapped gas curves, related to the synthesis of YBCO films by ion beam sputtering of elemental targets. The calculations are for Ar^{+}, Kr^{+}, and Xe^{+} ions impacting on Ba (a) and Cu (b) at normal incidence, with the substrate at 45°, as a function of kinetic energy of the primary ion.

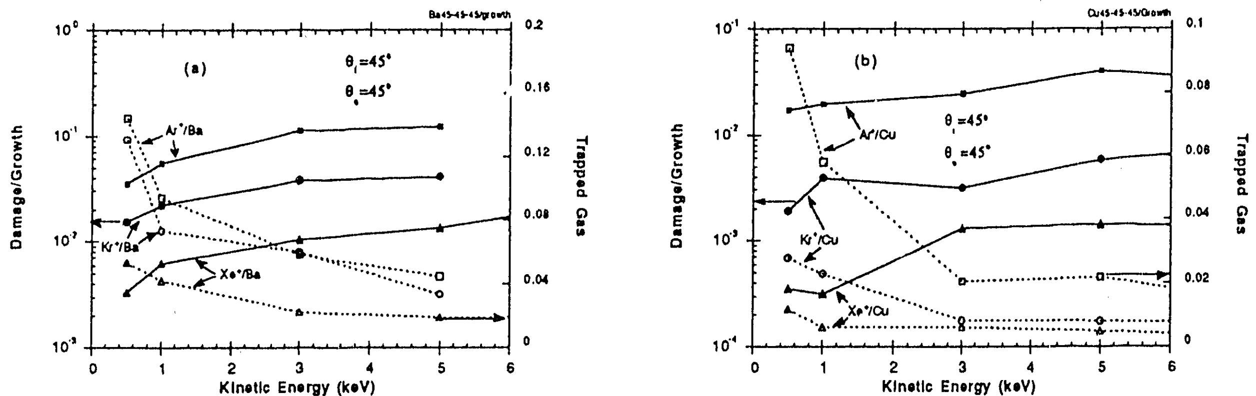

Figure 3. Normalized damage/growth and trapped gas curves, related to the synthesis of YBCO films by ion beam sputtering of elemental targets. The calculations are for Ar^{+}, Kr^{+}, and Xe^{+} ions impacting on Ba (a) and Cu (b) at 45°, as a function of the kinetic energy of the primary ion.

CONCLUSIONS

Computer simulations have been performed to calculate film deposition rates and erosion, damage, and gas trapping produced by scattered ions from elemental Ba, Cu, and Y targets used in ion beam sputter-deposition of Y-Ba-Cu-O superconducting thin films. The calculations presented in this paper were limited to damage and trapped gas in the films. The main conclusions are: (a) the heavier the primary ion used for sputtering the targets, the smaller the damage and the amount

of trapped gas in the films; (b) a normal or close to normal angle of incidence of the primary ion beam with respect to the target is the most favorable geometry to reduce ion scattering effects; (c) the damage produced in the growing films by the scattered ions may be the dominant mechanism for degradation of film properties, over that corresponding to gas trapping. However, further experimental work is necessary to confirm the applicability of the model presented here.

ACKNOWLEDGMENTS

The authors acknowledge the partial support by the U.S. Department of Energy, Office of Basic Energy Sciences under contract No. W-31-109-ENG-38, and by the Defense Advanced Research Projects Agency under contract N-00014-88-K-0525.

REFERENCES

1. O. Auciello, A.R. Krauss, A.I. Kingon, and M.S. Ameen, Scanning Microscopy, **4**, 203 (1990)
2. A. R. Krauss, O. Auciello, A. I. Kingon, M. S. Ameen, Y. L. Liu, T. Barr, T.M. Graettinger, S.H. Rou, C.S. Soble, and D.M. Gruen, Applied Surface Science, **46**, 67 (1990).
3. D.L. Lichtenwalner, R.Woolcott, C.N. Soble, S.H. Rou, O. Auciello, and A.I. Kingon, J. Appl. Phys, **70**, 1(1991).
4. J. Fujita, T. Yoshitake, and H. Igarashi, Appl. Phys. Lett. **56**, 295 (1990).
5. J.M. Grace, D.B. McDonald, M.T. Reitjen, J. Olson, R.T. Kampwirth, and K.E. Gray, J. Appl. Phys. **70**, 3867 (1991).
6. M. S. Ameen, O. Auciello, S. H. Rou, C. N. Soble, T. M. Graettinger, A. R. Krauss, A.I. Kingon, and M.A. Ray, Amer. Inst. of Phys. Conf. Proc. No. 200, 79 (1988).
7. P. F. Carcia and S. I. Shah, Appl. Phys. Lett. **56**, 2345 (1990).
8. A.S. Kao, C. Hwang, V.J. Novotny, V.R. Deline, and G.L. Gorman, J. Vac. Sci. and Technol. **A7**, 2966 (1989) .
9. T. Takagi, J. Vac. Sci. Technol. **A2**, 382 (1984).
10. M. Muroi, Y. Okamura, T. Suzuki, K. Tsuda, M. Nagano, and K. Mukae,Jap. J. Appl. Phys. Part 1, **29**, 69 (1990).
11. D.J. Lichtenwalner, C.N. Soble, R. Woolcott, O. Auciello, and A. I. Kingon (to be submitted to J. Appl. Phys., 1992).
12. J. P. Biersack and L.G. Haggmark, Nucl. Instr. Meth. **174**, 257 (1980).
13. O. Auciello and A.R. Krauss (to be submitted to J. Appl. Phys., 1992).

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

END

DATE FILMED

7 / 21 / 92