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MECHANISMS OF ION FORMATION IN LIQUID METAL ION SOURCES

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Résumé - Un modèle théorique sur les sources d'ions à métal liquide a été développé qui permet d'expliquer : 1) la forme et les dimensions de la zone émissive ; 2) les mécanismes de formation des ions ; 3) les propriétés du faisceau ionique. Cet article est principalement consacré au § 2). Nous montrons que l'évaporation de champ est le mécanisme dominant de l'émission ionique et que l'existence d'ions de charge double ou multiple provient d'un phénomène de post-ionisation. Ce modèle est ensuite utilisé pour étudier les propriétés du faisceau émis, telles que : l'intensité angulaire, le déficit et la largeur énergétique, l'abondance relative d'ions de différents états de charge.

Abstract - We have developed a theoretical model of Liquid Metal Ion Source (LMIS) operation to explain consistently; i) the shape and size of the ion emitting region, ii) the mechanisms of ion formation and iii) properties of the ion beam. In this paper we concentrate on ii), we find that field evaporation is the dominant ion formation mechanism and the occurrence of doubly or higher charged ions is attributed to a post-ionization mechanism. We discuss properties of the ion beams from LMIS such as angular intensity, energy deficit, energy spread and the relative abundance of different charge states in terms of our model of LMIS operation.

Liquid Metal Ion Sources (LMIS) are attracting increasing interest at the present time due to the potential applications of high-brightness, quasi-point source ion beams such as microfabrication and microanalysis. Many different liquid metals and alloys have been successfully used in LMIS and a variety of ions can be produced. As yet, however, theoretical understanding of the processes contributing to ion formation is incomplete. Indeed two notable discussions of the mechanism of emission from LMI sources by Gomer /1/ and by Prewett et al. /2/ disagree significantly in their conclusions.

Our objective is to construct a model of LMIS operation which gives a consistent picture of three different, but closely related, aspects of LMI sources:

i. The shape and size of the ion emitting region.
ii. The mechanism of ion formation.
iii. Properties of the ion beam.

In this paper we explain our model of LMIS operation with particular emphasis on the mechanisms of ion formation.

1. MECHANISMS OF ION FORMATION

The field evaporation mechanism of ion formation is shown schematically in fig. 1. An atom with binding energy H_o is field evaporated over a barrier of height Q(F) resulting in a singly charged ion. Higher charge states may subsequently be formed by post-ionization at position x_{pi} in fig. 1. Dixon et al. /3/ have suggested that by comparing observed ratios of doubly to singly charged ions in LMIS to calculated probabilities of post-ionization /4/ an estimate of apex field strength may be made. This possibility has been further considered by Kingham /5/ for various different LMI sources. Table 1 shows a comparison of the post-ionization model estimate of the apex field strength, F_{pi}, with an estimate, F_{ih}, for field evaporation of a singly charged ion based on the image-hump model. For most of the elemental ion sources in table 1 (Al, Ga, In and Bi) the values of F_{pi} and F_{ih} are in reasonable agreement and are all close to 2 V/Å. Elemental Au is an exception to this with F_{pi} = 3.5 V/Å which is in agreement with the observed low temperature evaporation field of Au, whereas the value of F_{ih} is known to be too high. In the case of the $Au_{90}Si_{10}$ alloy the F_{pi} values disagree, apparently in contradiction to the post-ionization model, but this is thought to be due to the formation of some Si^+ by field ionization. Field evaporation and subsequent post-ionization can produce charge states up to at least M^{3+} in some cases, whereas field ionization can only produce singly charged ions (with a negligible probability of subsequent post-ionization).

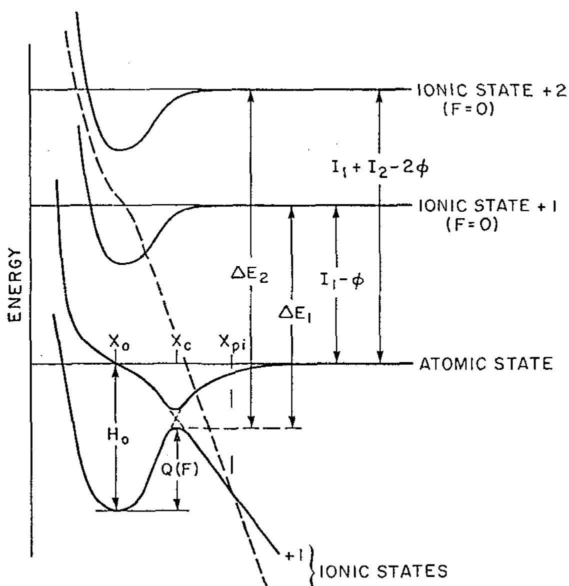

Fig. 1 - Potential energy diagram for field evaporation of a singly charged ion and possible post-ionization at x_{pi}. ΔE_1 and ΔE_2 are the ion energy deficits.

Table 1

Relative abundance of doubly to singly charged ions at 10 μA for various LMIS, observed by Swanson and co-workers. The calculated values of apex field strength based on the post-ionization model, F_{pi}, and the image-hump model, F_{ih}, are shown.

Elements in LMIS	Relative Abundance M^{2+}/M^{+} at 10 μA	F_{pi} (V/Å)	F_{ih} (V/Å)
Al	2.2×10^{-3}	2.0	1.8
Ga	9×10^{-5}	2.1	1.6
Ga(a)	-	1.9 - 2.0	1.6
In	2×10^{-5}	1.7	1.4
Au	1.5	3.5	5.1
Bi	2.3×10^{-2}	1.9	2.3
Si(b)	2.9	2.0	4.2
Au(b)	4.6	3.7	5.1
Y(c)	0.374(d)	2.1	4.2
Ni(c)	0.168	2.2	3.5

(a) estimate of F_{pi} taken from ref. 5

(b) results for an $Au_{90}Si_{10}$ alloy with F_{ih} based on pure metal values

(c) results for a $Y_{62}Ni_{23}B_{15}$ alloy with F_{ih} based on pure metal values

(d) relative abundance for Y is Y^{3+}/Y^{2+} not Y^{2+}/Y^{+}

Field evaporated ions have an energy deficit, ΔE, given by (see fig. 1)

$$\Delta E_n = H_o + \Sigma_n I_i - n \Phi_c - Q(F) \quad (1)$$

where Φ_c is the work function of the retarding elecrode and I_i is the ith ionization potential. This formula is appropriate to the post-ionization model of field evaporation as well as to the conventional image-hump and charge-exchange models. There is an intrinsic energy spread of about 1 eV due to variation in H_o between different evaporation sites and to thermal energy. The post-ionization process may introduce an extra broadening which should be less than 0.5 eV due to the finite width of the post-ionization zone /5/. The major cause of the observed energy broadening in an LMIS ion beam is a space charge effect of coulomb interactions between ions in the beam which results in a total energy spread which is usually observed to be at least 5 eV /6/. It has recently been pointed out by Gesley and Swanson /7/ that this effect also results in a mass and current dependent shift in the mean ion energy. Doubly charged ions are expected to have a reduced energy spread because they travel faster through the region of high space charge and the post-ionization mechanism has only a small extra broadening effect. This is in agreement with observation and it has important implications for fine focussed beam applications where the ion beam probe size is limited by chromatic abberation /8/. Doubly charged ions also give the advantage of doubling the available ion energy for a given voltage.

The possibility of developing ion sources specifically to give useful proportions of doubly and higher charged ions has been considered by Kingham /5/ following Van de Walle and Sudraud's observation of mainly U^{2+} and U^{3+} ions from a uranium LMIS /9/.

The jet-like protrusion model of LMIS shape (see section 2), which successfully overcomes Gomer's /1/ objection to a field evaporation mechanism of ion formation, does not eliminate the possibility of some contribution of field ionization to the total ion current. The temperature rise at the apex of such a shape is much greater than that for a truncated Taylor cone shape for a given heat input to the apex. Mair and Aitken /10/ have considered this for a Ga source and they suggest that thermal evaporation would be negligible. The present authors agree with this, but have found that for other elements thermal evaporation followed by field ionization may make a significant, but not dominant contribution to the total ion current. Field ionization, unlike field evaporation, can occur in a region many Å wide above the apex of the LMIS so that these ions have a broad energy distribution even before the effects of space charge. This may increase the overall energy spread of singly charged ions and can give rise to a two-peak or peak and shoulder structure in the energy distribution as has been observed for Ga^+ /11/ and for Si^+ /6/. Field ionization does not contribute to the current of doubly charged ions.

2. SHAPE AND SIZE OF THE ION EMITTING REGION

It was shown by Gomer /1/ that the usual assumption of a rounded off Taylor cone shape is inconsistent with a field evaporation mechanism of ion formation. Gomer interpreted his results as meaning that field evaporation could not be occuring at currents above 10 µA. An alternative view is that field evaporation is occurring, but that the shape is that of some jet-like protrusion on the end of a Taylor cone. We adopt this alternative view here, in agreement with Kang and Swanson's /12/ calculations and with the direct TEM observations of Gaubi et al. /13/.

3. CALCULATION OF PROPERTIES OF THE ION BEAM

We have made a self consistent calculation of LMIS shape and the ion trajectories including effects of space charge, using a modified version of the SCWIM program used by Kang and Swanson /12/. Examples of results of these calculations are given in figs 2 and 3. Fig. 2 shows that the calculated angular intensity as a function of beam

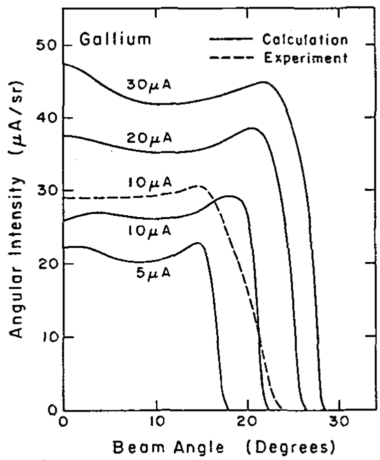

Fig. 2 - Comparison of calculated and measured angular intensity for a Ga source.

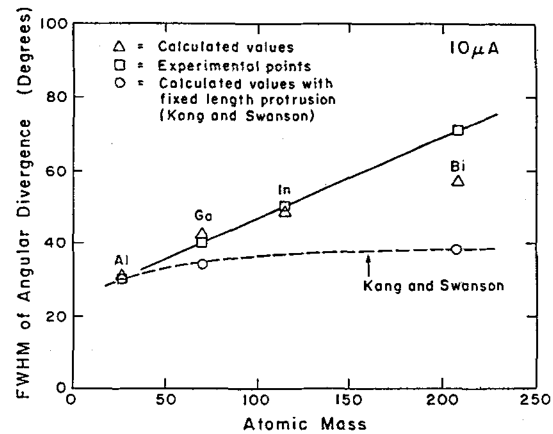

Fig. 3 - Comparison of calculated and experimental beam divergence at 10μA for different elements.

angle for a Ga LMIS is in resonable agreement with both the width and shape of the measured angular intensity. The FWHM of the angular intensity for different elements is shown in fig. 3. The results of the present calculation, which include a variable length protrusion on the end of a Taylor cone shape that adjusts to offset the effects of space charge, are in much better agreement with the experimental results than the fixed length protrusion model adopted by Kang and Swanson /12/.

4. SUMMARY AND CONCLUSIONS

A schematic view of Liquid Metal Ion Source operation is shown in fig. 4. The shape is that of a jet-like protrusion which assymptotically approaches a Taylor cone shape. The dominant mechanism of ion formation is field evaporation from the apex producing mainly singly charged ions, M^+, and perhaps some singly charged small clusters. A few Å from the tip the M^+ ions may, in some cases, be post-ionized to M^{2+} and subsequently to M^{3+} or even higher charge states. Small field evaporated clusters may also be post-ionized to higher charge states. A subsidiary mechanism of ion formation is field ionization of thermally evaporated neutral atoms and clusters. Polarization forces tend to attract these neutrals into the high field region above the apex where they may be field ionized at a distance of order 10 Å above the surface. This field ionization mechanism only gives rise to singly-charged ions.

Our conclusion is that the mechanism of ion formation in LMIS is predominantly field evaporation and that the source shape consists of a jet-like protrusion on the end of a Taylor cone shape, which grows steadily as the ion current increases.

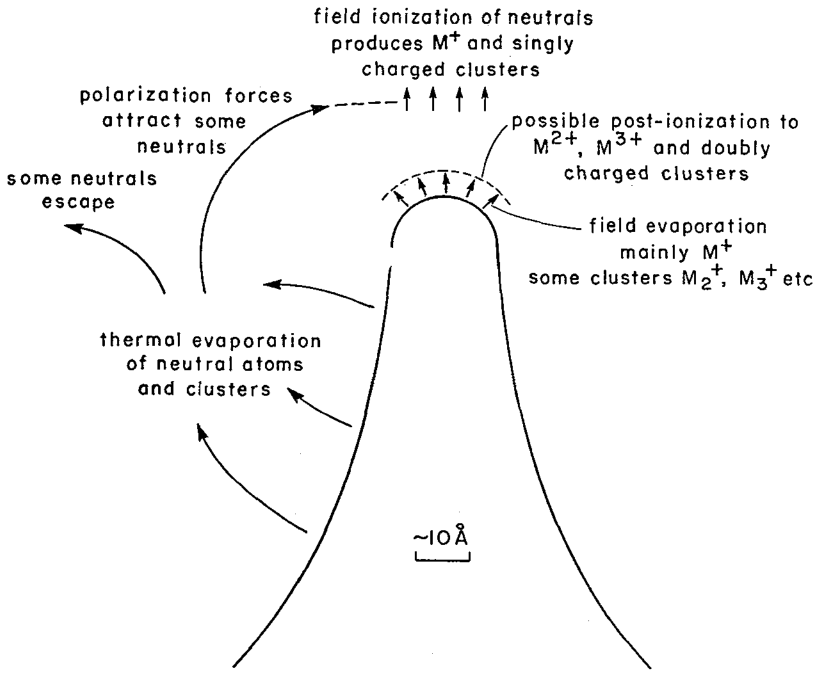

Fig. 4 - A schematic view of the present model of Liquid Metal Ion Source operation.

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