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Metal Atoms Trapped in Cryogenic Matrices as Potential Rocket Fuels

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Metal atom dispersions in cryogenic matrices are potential high-energy density rocket fuels. Using the I_{sp} extractable to rate a fuel, we have examined the potential of a family of "metal in matrix" fuels, in combination with liquid oxygen or liquid fluorine oxidizers. The fuels studied were composed of a dispersion of light metal atoms in a molecular hydrogen matrix. The I_{sp} was calculated using a thermodynamic code designed for rocket combustion. The code requires accurate values for the enthalpy of formation of the fuel ($\Delta H_{f(\text{fuel})}$). For any particular total metal mole fraction (i.e., loading) the metal in matrix fuel will contain a distribution of metal-bearing species. Each will have its own characteristic ΔH_f. The weighted sum of these yields $\Delta H_{f(\text{fuel})}$. Consequently, accurate calculation of $\Delta H_{f(\text{fuel})}$ requires that this population, the relative concentrations of free metal atoms, dimers, and metal bearing clusters, be accurately described. A statistical model was devised to predict this distribution. Using it, the enthalpy of formation of the fuel was computed. We find that several members of the family studied have, in combination with either liquid oxygen or fluorine, an I_{sp} potential significantly greater than that which characterizes the best currently available fuel/oxidized combination. In general, for all the family members studied, the maximum I_{sp} is extracted when the metal atom concentration is maximized, and under these circumstances the oxidizer reacts exclusively with the metal inclusions while the matrix behaves as the system's working fluid. Finally these predictions, based on our statistical model of the distribution of metal bearing species, were compared with predictions based on models in which 1) only metal atoms and dimers are present in the matrix, or 2) only selectively positioned metal atoms are included in the matrix.

Introduction

REACTIONS of low-mass metal atoms with liquid oxygen or liquid fluorine are highly exothermic. Their exothermicities are such that they represent a potentially significant improvement to the specific impulse I_{sp}, of available rocket fuels. Tapping this potential requires storage of the atom, but under conditions which largely leave its enthalpy unaffected. In a condensed medium this requires that interaction between the matrix and included atom be small. Cryogenic matrices can provide such a medium. The energy between the metal atom or any simple inclusion and the host material is expected to be relatively weak, and typified by the Van der Waal interactions which keep the matrix together. Experimental evidence supports this picture. The presence of only a weak host-guest interaction in such cryogenic matrices accounts for the close agreement between the electronic and vibrational spectra seen in species observed in the gas phase or trapped in matrices.[1,2]

Given an appropriate storage medium, the degree to which free metal atoms can be trapped becomes the most important gauge of how much specific impulse can be extracted from this kind of fuel. There is, however, a complication. It derives from the localization of the atom in the host matrix. As guest atom concentration in the matrix rises, the isolation of the guest atoms declines proportionately. There is a concomitant tendency for dimers to form. At higher loadings this drive will produce trimers and larger clusters. This limits the maximum free metal atom concentrations which can be attained, and in addressing the I_{sp} potential of the metal in matrix fuel, due allowance must be made for this polyatomic metal bearing component of the population and its thermodynamic properties.

These facts were recognized by researchers in the 1950s.[3] At that time, research efforts focused on schemes which would harness the energies of simple recombination reactions (e.g., $N + N \rightarrow N_2$), by trapping appropriate atom or free radical "guests" in a matrix. Such fuels would be monopropellants. Jackson and Montroll[4] calculated the maximum precursor concentration which could be trapped in in this way using a generating function technique. Their approach assumed that nearest neighbor guests would combine to form dimers, but that processes forming larger cluster species were absent. Consequently for an atom guest, the matrix, at all loadings, was populated by a distribution of atoms and diatoms only. They calculated that for a linear lattice as much as 17% of the guest population would exist as monomers, while in a three-dimensional crystal lattice approximately 10% of the precursors would remain uncombined. For metal in matrix fuels the situation is expected to be somewhat different. Unlike the situation dealt with in the Jackson and Montroll study in which the dimer product of precursor combination is presumed to be a very stable species with an essentially infinite barrier to further combination (e.g., $N_2 + N \rightarrow N_3$ is highly endothermic), there is no a priori reason to believe that the same is true for processes involving metal cluster formation.

In this report we describe a computational study of the I_{sp} potential of a family of metal in matrix fuels. The computation requires accurate values for the enthalpy of formation of the fuel [$\Delta H_{f(\text{fuel})}$]. Allowance is made for the distribution of different metal bearing species in the matrix through the use of a simple statistical model. With it we estimate the maximum metal atom precursor concentrations in situations where clustering continues beyond the dimer level. We assume that as long as metal bearing species occupy nearest neighbor positions in a crystal matrix, they bond to one another. In this simple model site statistics determine monomer, dimer, and higher order cluster concentrations for a given metal atom fraction. The energy intrinsic to the position of the atoms on the lattice sites introduces no bias in the statistics. In addition,

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the model assumes that both the matrix atoms (or molecules) and low mass metal atoms occupy only one site in the crystal. With this model we have calculated specific impulses (I_{sp}) for cryogenic fuels composed of low-mass metal atoms trapped in a hydrogen matrix when burned with either oxygen or fluorine. We conclude by noting that despite its simplifying assumptions, studies on model systems by Welker and Martin[5] and Presser et al.[6,7] have demonstrated that laboratory experimental conditions can be achieved in which the statistical model accurately predicts free metal atom levels in the matrix over the range of concentrations encompassed by our calculations.

Statistical Model

We begin by considering the preparation of a metal/matrix fuel, and idealize the process by treating it as a deposition in which a well-mixed gas stream containing metal atoms and a matrix species impinges on a cold surface. The species striking the surface are trapped at lattice sites associated with the surface and do not diffuse. It is assumed that there is no barrier associated with metal atom combination. Consequently, metal atoms occupying neighboring sites combine to form dimers, trimers, and higher order clusters. In addition, single occupancy is assumed with each lattice site occupied either by a metal atom or a matrix specie. The latter do not undergo any chemical transformations and only occupy sites. Thus, the deposited matrix is, except for the effects of the clustering process, representative of the random distribution present in the gas phase.

Monomers

The chance that a metal atom occupies any particular site is equal to the fraction f of metal atoms available. The chance that a matrix species occupies a particular site is $1 - f$. A metal atom surrounded by the matrix species at its nearest neighboring sites defines a monomer, i.e., a free-metal atom. The probability that a metal atom in the matrix exits as a monomer is

$$P_m = (1 - f)^n \tag{1}$$

where n is the number of nearest neighbors. Note that all the matrix atoms are indistinguishable. Only one configuration satisfies the monomer requirement that all nearest neighbor sites be occupied by matrix specie. As the fraction of metal atoms becomes diminishingly small, the probability that all the metal atoms exist as monomers approaches unit probability. The fraction of sites S_m which are occupied by metal atoms as monomers is

$$S_m = fP_m = f(1 - f)^n \tag{2}$$

The maximum number of sites which can be occupied by a metal monomer can be derived by differentiating Eq. (2), setting it to zero, and solving for f. The fraction of metal atoms which produce the maximum number of monomers sites is

$$f_m(\max) = 1/(n + 1) \tag{3}$$

and this maximum value is presented in Table 1 for various lattice structures. The fraction of sites occupied by isolated metal atoms is equivalent to the mole fraction $X_m(\max)$ of metal monomers.

Dimers

A similar construction may be applied to dimer formation. A dimer is one in which one of the nearest neighbors of a selected metal is another metal atom while all other sites surrounding the couple are occupied by matrix species. The probability that the nearest neighbors of a selected metal atom A, are one metal atom A', with the remaining nearest neighbor sites occupied by indistinguishable matrix atoms or molecules, is $nf(1 - f)^{n-1}$. The multiplicative factor n represents the number of ways (configurations) to position the second metal atom. Therefore, compound probability P_d for dimer formation as a function of the fraction of metal atoms present is

$$P_d = nf(1 - f)^{n-1}(1 - f)^{n-s-1} \tag{4}$$

The last factor in the expression is the probability that nearest neighbor sites about A' are occupied by matrix species (exclusive of the first metal atom). The exponent s discounts the number of nearest neighbor sites shared by both metal atoms, since these are already allowed for in the first term of the expression. The fraction of sites S_d which are occupied by metal atoms in the form of dimers is

$$S_d = fP_d = nf^2(1 - f)^{2n-s-2} \tag{5}$$

The maximum number of sites occupied by a metal dimer (consisting of two sites for a dimer) can be derived by differentiating Eq. (4), setting it to zero, and solving for f. The total metal-atom fraction which maximizes the number of dimer sites is

$$f_d(\max) = 1/[n - (s/2)] \tag{6}$$

The mole fraction X_d of dimers is equal to one-half of the fraction of lattice sites occupied by metal atoms in the form of dimers. Table 2 presents a listing of the metal atom fraction which produces the maximum dimer mole fraction for the four crystals.

Higher Order Clusters

Calculating the probability for a given atom to appear in the form of a trimer and higher order cluster is also straightforward, but requires determining various possible configurations and summing them. For example, the three metal atoms in a trimer can share mutually nearest neighbor sites with a unique number of shared sites containing matrix species. On the other hand, a second configuration is possible. The metal atoms would have two metal atoms as a nearest neighbor. In this latter case, the number of shared nearest neighbor sites differs from the first case. For this report, however, we need consider only the monomer and dimer concentrations in determining the available energy content of the crystal. We have assumed that the energy content of trimers and higher order clusters is that of the bulk metal in its standard state. This assumption underestimates the stored energy content of the matrix.

I_{sp} Calculations

Using this model for estimating maximum monomer concentrations, we have calculated the I_{sp} for various fuel/oxidizer

Table 1 Maximum monomer concentrations for various crystals

Crystal	n	$f_m(\max)$	$X_m(\max)$
Simple cubic	6	0.143	0.067
Body centered cubic (bcc)	8	0.111	0.049
Face centered cubic (fcc)	12	0.077	0.032
Hexagonal closed packed (hcp)	12	0.077	0.032

Table 2 Maximum dimer concentrations for various crystals

Crystal	n	s	$f_m(\max)$	$X_m(\max)$
Simple cubic	6	0	0.167	0.0135
Body centered cubic (bcc)	8	0	0.125	0.0096
Face centered cubic (fcc)	12	4	0.100	0.0090
Hexagonal closed packed (hcp)	12	4	0.100	0.0090

Table 3 Heats of formation (kcal/mole) and densities for reactants in the I_{sp} calculation[10]

Atom	ΔH_f Monomer	ΔH_f Dimer	Density, g/cm^3
Li	37.69	51.50	0.53
Be	76.42	150.83	1.85
B	132.62	196.78	2.34
C	169.98	198.20	2.62
Na	25.69	34.56	0.97
Mg	34.77	68.88	1.74
Al	78.23	116.22	2.70
Si	106.52	140.32	2.62

mixtures. The fuel consists of metal atoms trapped in a molecular hydrogen matrix, and the oxidizer is either liquid oxygen or liquid fluorine. Estimates for the heat of formation of the individual metal in matrix fuels are obtained by summing the heats of formation of the individual components weighted by their mole fraction in the matrix

$$\Delta H_{f(\text{fuel})} = \sum_i w_i \Delta H_{f(i)} \tag{7}$$

where w_i is the mole fraction for each component. In these calculations we assume that total metal-atom mole fraction in these calculations is 0.077. This fraction of metal atoms provides the greatest monomer concentration as calculated by our model for a hexagonal-close-packed lattice, which is the normal crystal structure for solid hydrogen (Table 1). Of the metal-atoms present in the fuel, 38% are monomers and approximately 7% are dimers. The remaining metal-atoms in the form of trimers and higher order clusters are treated in the calculation as solid metal in its standard state. Table 3 lists the heats of formation and densities for the oxidizers, hydrogen host, and low-mass atoms and dimers used in the I_{sp} calculations.

The Edwards Air Force Base EDCONVU[8] code used in this study is an equilibrium code which calculates the I_{sp}, temperature, and concentration of product species at the rocket exit plane. Throughout these calculations we have assumed a chamber pressure of 1500 psi, and no effort was made to optimize the I_{sp} results by varying this parameter. The exhaust pressure was taken as 14.7 psi. The results of a calculation for the reaction of neat hydrogen with oxygen or fluorine serve as our baseline, and 1 mole of hydrogen corresponds to the stoichiometric consumption of either oxidant, if no metal is present.

While we describe the results for selected systems in the ensuing section, certain general trends in our results should be noted. In particular, for all the systems studied, the metal additive reacted preferentially with the oxidizer. At very low fuel/oxidizer (F/O) ratios, the metal additive and the matrix H_2 were consumed. The very low F/O region is characterized by the high temperatures of the H_2 + Oxidant reaction and dominated by its chemistry. As F/O ratios increase, it is the metal bearing species which are consumed in preference to H_2. This tendency continues until a F/O ratio is reached, where sufficient metal atoms are available for the stoichiometric consumption of the oxidant. At that point, the H_2 in the matrix fuel does not partake in the combustion chemistry, but becomes the system's working fluid. This shift in consumption from the hydrogen to metal atom has other consequences; the most important is the significant reduction in the exhaust temperature. The lower exhaust temperatures allow some of the primary reaction products to condense out as solids, with a concomitant release of heat of condensation which increases the I_{sp} extracted from the system.

Lithium

Figure 1 is a summary of the results for a lithium/hydrogen (0.077/0.923) metal/matrix fuel in combination with liquid oxygen. As previously indicated, our baseline is the combustion of pure hydrogen with oxygen. Here, and in subsequent figures, our results are plotted as a function of "moles of hydrogen" present in the initially reacting mixture. This allows direct comparison with the baseline system. Stoichiometry is achieved with 1 mole of hydrogen (i.e., 0.5 moles of molecular oxygen are available for consumption). At its peak, the addition of lithium atoms to the matrix provides a 4% increase in the extracted I_{sp}. The improvement in the I_{sp} is very gradual, making this quantity only weakly dependent on the exact F/O ratio. This is in marked contrast with the baseline reaction system where there is a rapid decline in the I_{sp}, once the optimal F/O ratio is attained. This behavior extends to F/O ratios as high as 20. The maximum I_{sp} is attained at a F/O ratio of 7.5, which corresponds to a Li/O_2 ratio of about 1:1. The increase in I_{sp} for the higher F/O mixtures is due in large part to the extraction of the condensation energy associated with the major lithium products, LiOH and Li_2O. The throat temperature decreases as the F/O ratio increases.

Burning this same lithium/hydrogen (0.077/0.923) fuel with fluorine produces much the same result. In these calculations, 1 mole of fluorine oxidizes 1 mole of hydrogen at the stoichiometric point. Figure 2 shows the I_{sp} and temperature var-

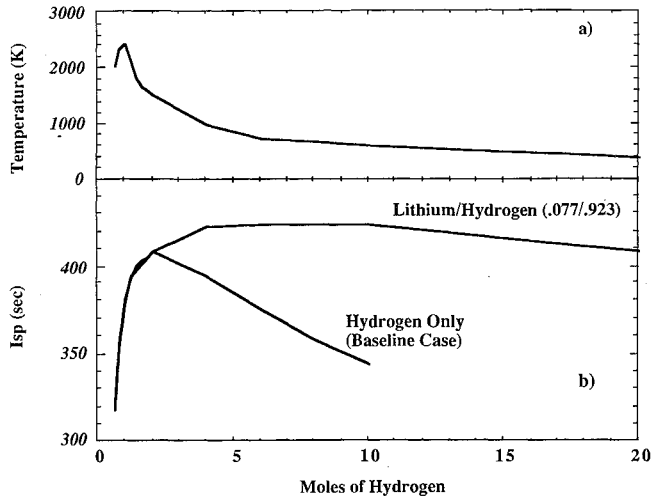

Fig. 1 Computed results for the combustion of a lithium/hydrogen (0.077/0.923) matrix fuel with 0.5 mole liquid oxygen: a) exit plane temperature and b) I_{sp}. P(combustion chamber) = 1500 psi, P(exit plane) = 14.7 psi.

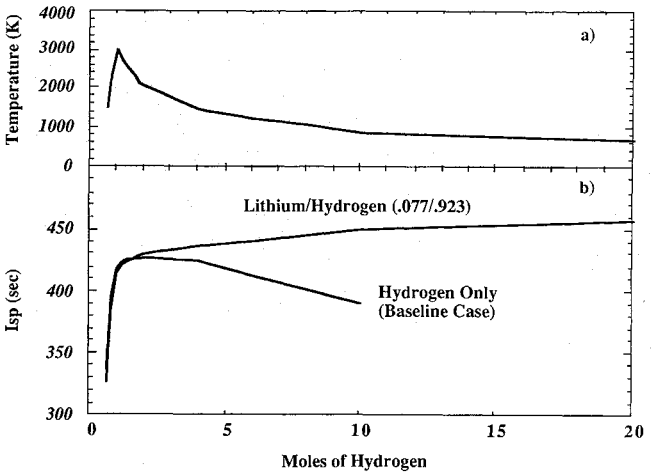

Fig. 2 Computed results for the combustion of a lithium/hydrogen (0.077/0.923) matrix fuel with 1.0 mole liquid fluorine: a) exit plane temperature and b) I_{sp}. P(combustion chamber) = 1500 psi, P(exit plane) = 14.7 psi.

iation in this system. Results are plotted as function of moles of hydrogen in the matrix fuel for direct comparison to baseline $H_2 + F_2$ reaction. As in the case of oxygen, the condensation and freezing of LiF at higher *F/O* ratios releases additional energy. The improvement in the I_{sp} for this reaction system is approximately 7%.

Boron

In a similar calculation, we determined the temperatures and I_{sp} for a boron/hydrogen (0.077/0.923) matrix fuel. Figure 3 shows the results for this calculation. The combustion products in this reaction are more diverse than for lithium combustion. Despite this, the same basic trend is observed. In this reaction system too, the temperature peaks at low *F/O* ratios and the chemistry is dominated by the $H_2 + O_2$ reaction. The exhaust temperature decreases significantly as the *F/O* ratio increases. The I_{sp} for a boron/hydrogen matrix peaks at a value of 476 s, an increase of 16% over the baseline $H_2 + O_2$ reaction. The major reaction product is B_2O_3, which condenses at the lower exhaust temperatures, releasing additional energy.

Burning a boron/hydrogen fuel with fluorine does not provide as large a fractional improvement in I_{sp} when compared to its baseline $H_2 + F_2$ reaction. As the *F/O* mixture increases, the exhaust temperature does decrease. However, the major combustion product in this system is BF_3, which is volatile and does not condense despite the lower nozzle temperatures. In this reaction system the addition of boron increases the I_{sp} only 11% as shown in Fig. 4.

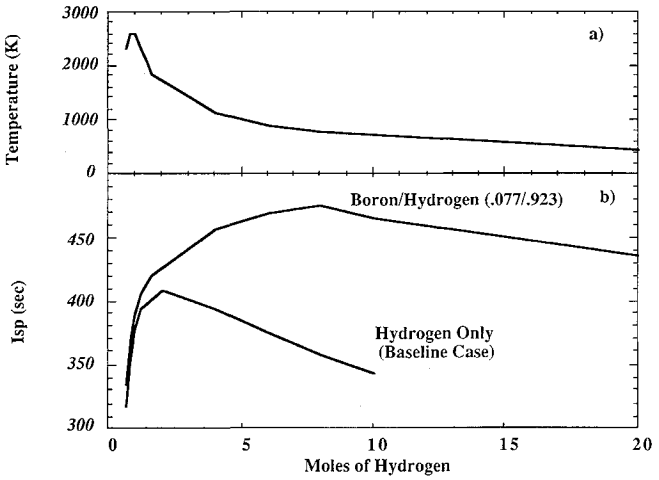

Fig. 3 Computed results for the combustion of a boron/hydrogen (0.077/0.923) matrix fuel with 0.5 mole liquid oxygen: a) exit plane temperature and b) I_{sp}. *P*(combustion chamber) = 1500 psi, *P*(exit plane) = 14.7 psi.

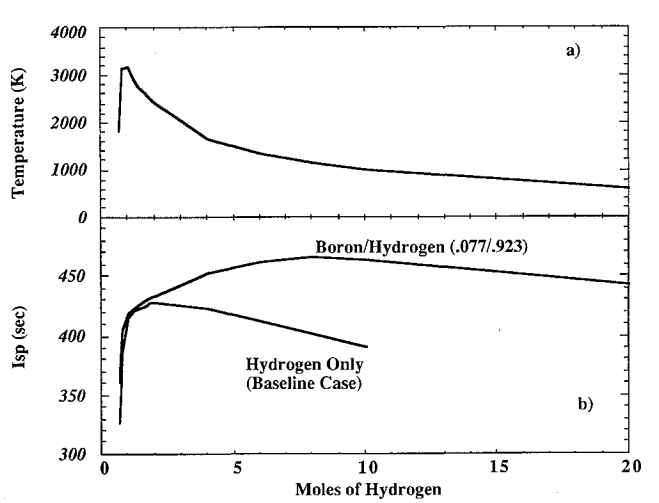

Fig. 4 Computed results for the combustion of a boron/hydrogen (0.077/0.923) matrix fuel with 1.0 mole liquid fluorine: a) exit plane temperature and b) I_{sp}. *P*(combustion chamber) = 1500 psi, *P*(exit plane) = 14.7 psi.

Table 4 Peak I_{sp} calculated for hydrogen containing 7.7% metal atom additive reacting with oxygen and fluorine

Fuel additive	Oxidizer: Oxygen I_{sp}, s	Oxygen: Major products	Fluorine I_{sp}, s	Fluorine: Major products
None	404	H_2O	424	HF
Li	404	Li_2O(c)	457	LiF(c)
Be	490	BeO(c)	466	BeF_2(l)
B	476	B_2O_3(c)	463	BF_2
C	435	CO, CO_2, H_2O	440	CH_4, HF
Na	378	Na_2O(c)	413	NaF(l)
Mg	414	MgO(c)	436	M_gF_2
Al	438	Al_2O_3(c)	428	AlF_3
Si	437	SiO_2(c)	432	SiF_4

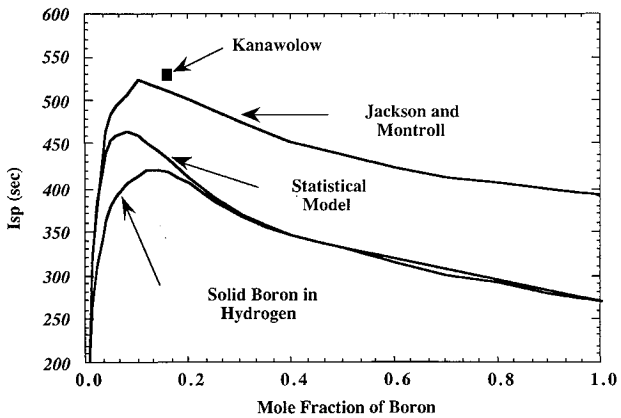

Fig. 5 Calculated dependence of I_{sp} on the mole fraction of boron in boron/hydrogen matrix fuel. Metal population in fuel 1) given by statistical model, 2) only solid boron, 3) contains only atoms and diatoms (J&M), and 4) contains energy optimized nonrandom boron/hydrogen clusters.

Table 4 lists the results of the I_{sp} calculations for other composite fuels consisting of low mass metal atoms trapped in hydrogen matrices and reacting with either oxygen or fluorine. In addition to the peak I_{sp} reported, Table 4 includes the major products generated at the peak I_{sp}. Beryllium produced the highest I_{sp} followed by boron. Carbon was the only atom which did not preferentially react with the oxidizer. In burning oxygen with the hydrogen/carbon mixture, the major products producing the maximum I_{sp} were CO and CO_2. Increasing the *F/O* ratio, however, produced methane and water. The reaction of H_2/C with fluorine at the maximum I_{sp} produced methane and HF.

In the calculations described above, it was tacitly assumed that the maximum I_{sp} would be extracted when the concentration of free metal-atoms was maximized. To test this hypothesis, a set of calculations was performed in which the metal loading (and consequently, the population of free metal-atoms in the matrix) was varied. The fuel was a boron/hydrogen matrix, and the calculations used the monomer and dimer concentrations predicted by the statistical model. Stoichiometric amounts of oxidizer were used to react all the metal present in the matrix. Hydrogen remained unreacted acting as a coolant. At low metal atom fractions the calculations show that the temperature at the nozzle is low and increases as the metal mole fraction increases. Figure 5 shows how the I_{sp} varies as the total boron mole fraction trapped in hydrogen increases. The peak I_{sp} value does indeed correspond to the maximum monomer concentration of 7.7%.

Conclusions

The results we have presented indicate that a number of metal/matrix fuel systems may be able to provide I_{sp} greater than those available from the $H_2 + O_2$ or $H_2 + F_2$ reactions. In a number of instances this improvement is significant. In addition, it is important to recognize that these estimates are conservative, insofar as they depend on our statistical model which permits only monomers and dimers to contribute to I_{sp} enhancements, all other metal bearing species being treated as bulk material. The potential enhancement from the latter in the boron/hydrogen matrix system is also depicted in Fig. 5.

It is interesting to consider how the statistical model's assumptions impact the I_{sp} which may be extracted from the metal matrix fuel. In particular, we need to consider what might be the potential extracted from such a system under two extreme conditions. The first is analogous to the J&M model in which only atoms and diatoms populate the matrix, although still in a statistical manner, and the second is one in which a nonstatistical, ordered highest energy crystal structure is imposed on the metal/matrix. This is not simply an exercise, since it is possible that free-metal atom concentrations in a matrix will exceed our model's predictions. Our model assumes no activation energy to the formation of trimers, tetramers, or higher order clusters. For example, in the lithium or boron systems, the formation of the dimer has no activation barrier and proceeds at any temperature. The formation of a trimer from a monomer and dimer, however, may have an activation barrier which greatly exceeds the available thermal energy, kT_{matrix} (approximately 5.75–28.75 cal/mole for a hydrogen-based matrix system). Processes which may proceed with alacrity at room temperature or higher, will be severely inhibited. The presence of such a bottleneck would halt the clustering process, leaving a matrix populated predominantly by atoms and diatoms. Under these conditions we recover the monomer and dimer distributions predicted by the J&M analysis. The I_{sp} calculated for the boron/hydrogen matrix fuel, obeying those statistics, is shown in Fig. 5. The results make it evident that the presence of barriers in the sequence of reactions leading to cluster formation can have a profound impact on the I_{sp}, which can be extracted from these types of fuels. In the boron/hydrogen system, the maximum I_{sp} approaches 550 s, nearly a 30% improvement on the $H_2 + O_2$ system.

Do these results differ from those for an ordered metal/matrix crystal which would contain the maximum number of free metal-atoms? Results for this kind of system would set the upper bound to the I_{sp}, which could be extracted from a particular metal/matrix system. Kanawolow[9] has calculated the Van der Waals interaction energy (~40 cm^{-1}) between lithium and hydrogen, and shown that the preferred (lowest energy) matrix/metal cluster would involve a central lithium atom surrounded by six hydrogens, four equatorial hydrogens, and two in an axial position. Assuming the boron-hydrogen interaction will impose a similar lowest energy configuration, the maximum I_{sp} which may be extracted from such a matrix is greater yet, as shown in Fig. 5. Interestingly, this upper bound on the I_{sp} is only a small fractional improvement when compared to the J&M-type matrix.

Acknowledgment

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