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The retardation of dissolution of Al-SiC composites in acidic medium-A green approach

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Abstract

The retardation of dissolution of Al-SiC composites in 1N HCl could be studied by using sulfaguanidine drug (SGD) as a green corrosion inhibitor . The performance of the compound has been explored using mass loss studies , gasometric measurements , potentiodynamic polarization and impedance analysis. These studies evidently pointed out that the compound performed as cathodic inhibitor in 1N HCl. The adsorption of the drug molecule on Al-SiC surface followed Temkin's adsorption isotherm. The quantum mechanical calculations validated the inhibition efficiency of the compound studied by electrochemical methods.

Keywords : Corrosion inhibitor, sulpha drugs , quantum , Adsorption

Introduction

Metal matrix composites (MMC) are widely as an alternate candidate to conventional materials for the manufacturing of high utility materials. The materials which are fabricated from metal matrix composites exhibited better mechanical properties than conventional materials due

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to its distinctive profile that can be used in machineries after compacting and sintering MMC's at optimized conditions. In the present study , Aluminium (AA 6061) and SiC powders were used as matrix and reinforcement (SiC) to prepare Al-SiC composites . Even though the so obtained Al-SiC offered enhanced tensile strength ,thermal expansion and wear resistance, when these materials are come in contact with aggressive environment, worn of machine parts occurs due to the dissolution of composites by attack of chloride ions. Numerous investigations have been carried out to decrease the corrosion of metals in aggressive and sea water environments. Among them, the use of eco friendly corrosion inhibitors is a study of recent trend . Thiourea and its derivatives have been reported as good corrosion inhibitors for mild steel and aluminium[1-5] in acidic and neutral media . According to Eno etal [6] and Shukla [7] , two antibiotic drugs viz., sparflaxin and cefalexin were identified as impressive inhibitors for the corrosion of mild steel in acidic media. Karthikeyan and his co investigators [8-10] have studied the influences of cloxacillin , ampicillin drugs ,furosemide and torsemide as corrosion inhibitors of mild steel in acidic media. Recently Umasankar et al [11] have investigated the influence of aminosulphaacetamide on the corrosion of Al-SiC composites in 1N HCl.

The ability of the compound to perform as potential inhibitor depends on its molecular structure , localization of electrons and electron releasing moiety. This paper describes the effect of a ecofriendly drug molecule , sulpha Guanidine (SGD) on the dissolution of Al-SiC composites in 1N HCl medium using mass loss studies , gasometric measurements, potentiodynamic polarization and impedance analysis. Quantum mechanical calculations have been carried out to justify the inhibition performance of the drug molecules in corrosive medium.

Experimental methods

Al-SiC composites were obtained from AA 6061 which had the compositions , Fe = 0.19%, Cu = 0.27%, Si = 0.56%, Zn = 0.03%, Mg = 0.94% and Al remainder, and of size 2 cm x 1 were used for mass loss

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and gasometric measurements . The mass loss study was carried out at room temperature for three hours in 1N HCl. The inhibition efficiency (IE %) was determined by the following equation, I.E (%) = (W –Wi /W) X 100

Where W & Wi are the mass loss values in the absence and presence of the drug molecule. Al–SiC cylindrical rod of the same composition as mentioned and fitted tightly in araldite resin with an exposed area of 1cmx 0.5 cm was used for potentiodynamic polarisation , hydrogen permeation and AC impedance studies. A platinum foil with surface area of 30 mm^2 and $Hg/Hg_2Cl_2/KCl_{(satd)}$ were employed as auxiliary and reference electrodes for electrochemical evaluations using EG&G Princeton Applied research model 7310. The quantum mechanical indices like HOMO, LUMO, energy gap and dipole moment of the compound were studied with aid of Gaussian software .

Results and Discussion

Mass loss and gasometric measurements:

The results of mass loss and gasometric studies are presented in table 1. It can be that the dissolution of composite in 1N HCl is retarded by addition of increased concentration of drug molecule. The maximum corrosion inhibition was achieved at 60 ppm of inhibitor ,beyond this; a decreased trend in inhibition was noticed due to peel off of inhibitor. The higher inhibition efficiency of the compound can be attributed to its adsorption on the surface of the metal matrix composite.

Potentiodynamic polarization studies:

The polarization studies have been carried out potentiodynamically at sweep rate of 1 Mv/sec with and without inhibitor for the corrosion of metal matrix composites in acidic medium. According to this study, the inhibitor reduced the composites dissolution which is evidenced from the decreased values of both corrosion potential (E_{corr})and corrosion

ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

current(I_{corr}) in 1N HCl. The anodic and cathodic Tafel slopes have been shifted to more positive directions equally in the presence of inhibitor , however the values of b_c are enhanced to greater a extent. So the dissolution of Al-SiC composites in acidic medium is under cathodic control which are in given as Tafel plot (Figure 1). These results are in good consistency with weight loss and gasometric studies.

Impedance studies:

The impedance curves for the corrosion of Al-SiC composites in the presence and absence of different concentration of drug molecule are given in table 3. It is evident from figure 2 that perfect semicircles were obtained for the corrosion inhibition process representing that the reaction follows charge transfer mode. The formation of semi circle at low frequency end related to composite dissolution whereas at frequency end indicated the formation of inhibitor film on the surface of Al-SiC composites. The charge transfer resistance was found as high and it attained maximum value at 60 ppm of drug molecule ,where as double layer capacitance values was brought down with increased concentrations of inhibitor [12]. This could be due to the effective adsorption of the compound on the surface of Al-SiC composites.

Hydrogen permeation measurements

The results of hydrogen permeation measurements obtained for the corrosion of composites in the presence and absence of the inhibitor in acidic medium are presented in Table 4. Due to , aggressiveness of chloride ions , the composite dissolution is high in 1N HCl in the absence of inhibitor. Eventhough SGD retarded the corrosion of Al-SiC in acidic medium, it enhanced the ingress of hydrogen due to its decomposition on composite surface [13] and thus evolving H_2S gas as reported by Lane etal[14] . The whole process takes place in two steps. In the first step, Sulpha guanidine molecules are adsorbed on Al-SiC surface through the anchoring of lone pairs of electrons of nitrogen and

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sulfur atoms. In the second step, the adsorbed inhibitor, may gradually undergo chemical changes. It is imperative fact that , the sulphur containing inhibitor decompose by forming H_2S due to the evolution of hydrogen gas which is evolved on the surface of Al-SiC, when exposed in 1N HCl. The plot of surface coverage (Ø) Vs log C gave straight line indicating that adsorption of by sulphaguanidine molecule on the surface of Al-SiC composites obey Temkin's adsorption isotherm.

Quantum mechanical studies:

The computed quantum mechanical indices such as energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), LUMO- HOMO, energy gap (ΔE), dipole moment (μ), are reported for SGD molecule in Table 5. The HOMO and LUMO distribution on amino ,imino moiety (Figure 3-5) is higher than sulphoxide groups of the inhibitor. It has been well established that, higher the value of E_{HOMO}, greater is the ease for the compound to release electrons to unoccupied d orbital of aluminium atom and higher is the inhibition efficiency. Further lower the E_{LUMO}, easier is the withdrawl of electrons from aluminium metal to form feedback bonds. The gap between HOMO-LUMO energy levels of molecules validates the adsorption of inhibitor. Higher , the values of energy gap of an inhibitor and dipole moment , higher is the inhibition efficiency of that molecule [15].

Conclusions

1. The mass loss and gasometry studies indicated that sulphaguanidine retarded the dissolution of Aluminium composites efficiently in 1N HCl.

2. The inhibition of corrosion of composite in 1N HCl , by the drug molecule followed cathodic control reaction.

ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

3. Impedance parameters calculated for the corrosion of composites in acidic medium justified the impressive performance of the compound.

4. The compound is found to enhance the ingress of hydrogen through Al-SiC surface by forming H_2S gas.

6. The quantum mechanical studies validated the efficient performance of inhibitor for Al-SiC composites dissolution in acidic medium.

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JCSE The Journal of Corrosion Science and Engineering
ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

Table 1. Values of inhibition efficiency for the corrosion of Al/SiC composites in 1N HCl in the presence of different concentrations of SGD obtained from weight loss and gasometric measurements.

Concentration of Inhibitor (ppm)	Inhibition efficiency (%)	
	Weight loss Studies	Gasometric measurements
Blank	---	---
20	76	75.6
40	87	86.5
60	94	93.8

ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

Table 2: Corrosion kinetic parameters of Al/SiC composites in 1N HCl in the presence of different concentrations of SGD obtained from potentiodynamic polarization studies.

Con. SAM	E_{corr} (mV vs SCE)	I_{corr} (µA cm-2)	b_a (mV dec-1)	b_c (mV dec-1)	IE (%)	θ
Blank	-484.00	553.13	88.4	146.6	-	-
20 PPM	-458.17	143.64	72.9	132.31	74.03	0.74
40 PPM	-383.43	82.17	59.4	103.62	85.14	0.85
60 PPM	-343.27	41.19	52.4	81.65	92.6	0.93

Table 3.Impedance values for the corrosion of Al/SiC composites in 1N HClin the presence of different concentrations of SGD.

Concentration of Inhibitor (ppm)	1N HCl solution	
	Charge Transfer resistance (R_{ct}) Ohm.cm^2	Double layer capacitance (C_{dl}) µF.cm^{-2}
Blank	43.6	162.8
20	132	65.4
40	158.2	43.2
60	175	23

JCSE The Journal of Corrosion Science and Engineering
ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

Table 4. Values of permeation current for the corrosion of Al/SiC composites in 1N HCl in the presence of different concentrations of SGD.

Concentration of Inhibitor (mM)	Steady state permeation current (μA)
	1N HCl
Blank	24.6
20	27.2
40	33.4
60	41.5

JCSE The Journal of Corrosion Science and Engineering
ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

Table 5: Quantum mechanical parameters for the inhibitor

Compound	LUMO (eV)	HOMO (eV)	ΔE (Cal.Mol^{-1})	Dipole moment (Debye)
Sulphaguanidine [SGD]	-1.695	-10.858	9.163	5.021

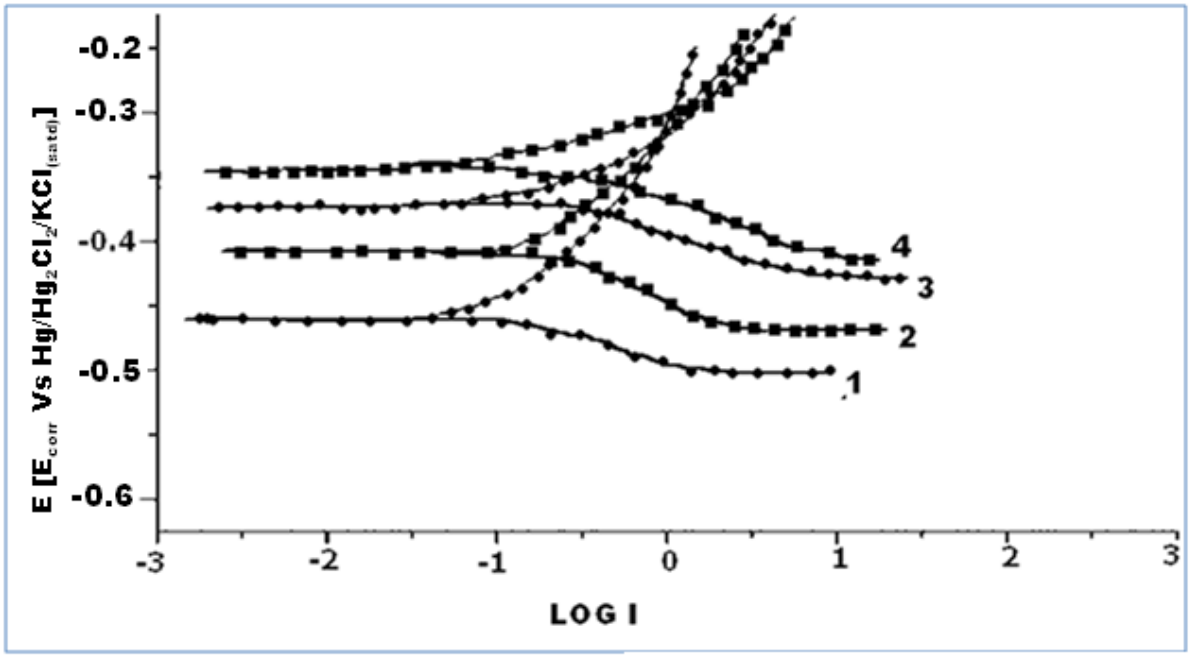

Figure 1

1. Blank ; 2. 20 ppm ; 3. 40 ppm; 4. 60 ppm

ISSN 1466- mitted 29 June 2013

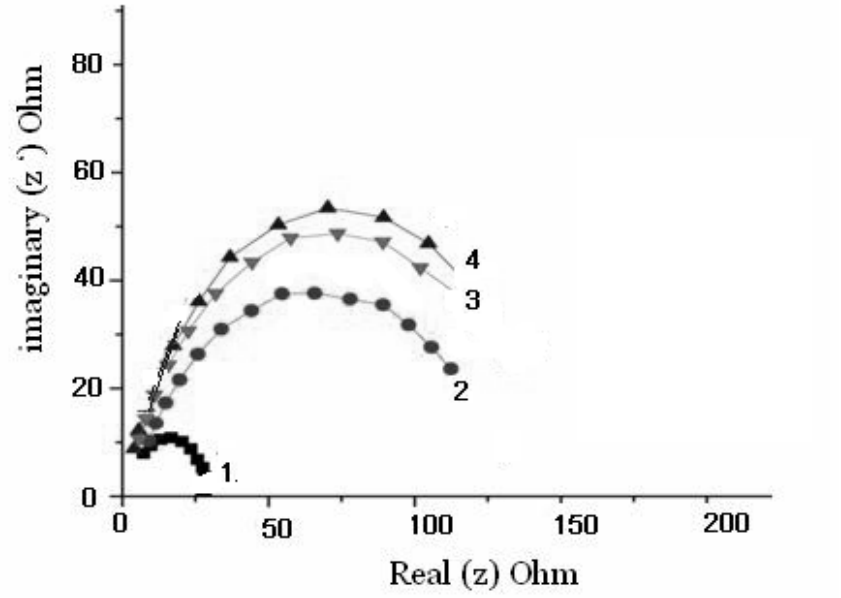

Figure 2.

1. Blank ; 2. 20 ppm ; 3. 40 ppm; 4. 60 ppm

JCSE The Journal of Corrosion Science and Engineering
ISSN 1466-8858 Volume 16, Preprint 45 submitted 29 June 2013

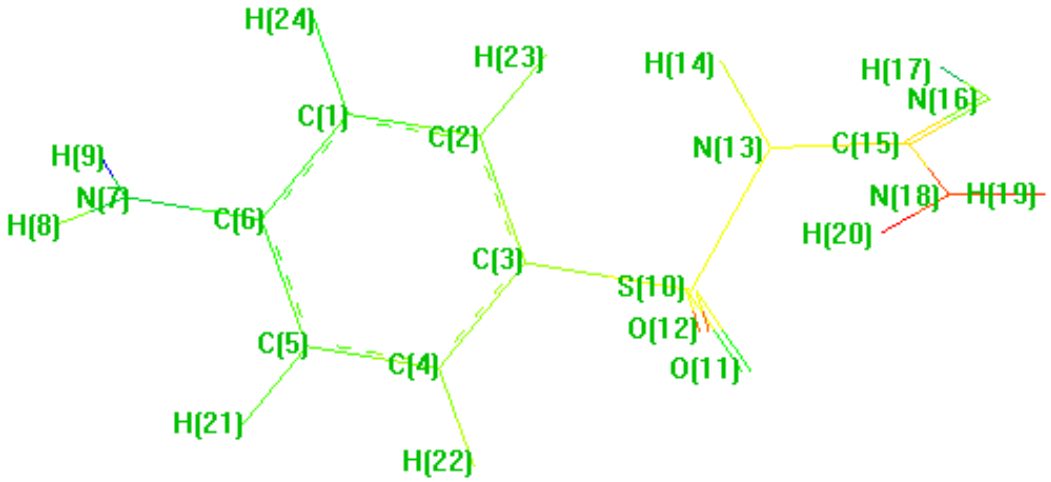

Figure 3

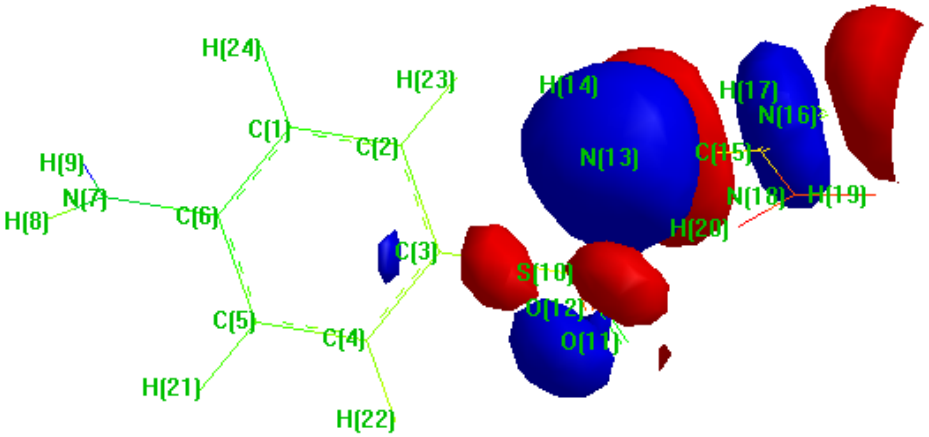

Figure 4

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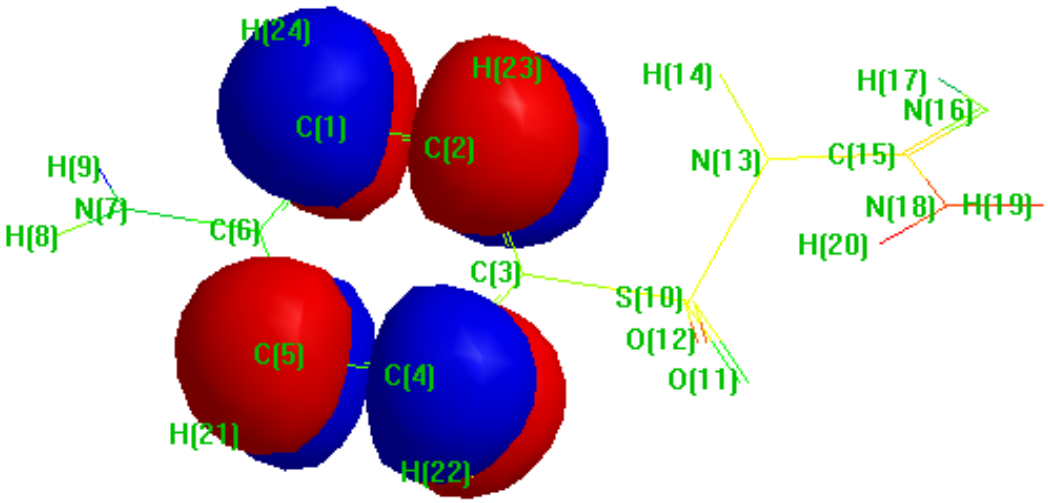

Figure 5

Legends for figure

1. Potentiodynamic polarization plot for Al-SiC composites in 1N HCl with different concentrations of inhibitor.
2. Impedance curves for the corrosion of aluminium composites in 1N HCl in the presence and absence of SGD.
3. Optimized structure of SGD (Wire frame model).
4. Highly occupied molecular orbital (HOMO) for SGD .
5. Lowest unoccupied molecular orbital (LUMO) for SGD.