NONLINEAR FEEDBACK CONTROL OF A COUPLED KINETIC MONTE CARLO-FINITE DIFFERENCE CODE

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Abstract: Product quality variables for many electronics and materials processes are set at the nanoscale and smaller length scales. Although the control of these processes is of scientific and industrial interest, there is a shortage of feedback controller design methods based on the noncontinuum models that describe such nanoscopic phenomena. In this study, linear, gain-scheduled, and nonlinear feedback controllers are designed for a coupled kinetic Monte Carlo-finite difference code that simulates the manufacture of copper interconnects. The feedback controller designs incorporate a low order stochastic model constructed from the coupled continuum-noncontinuum code.

Keywords: Stochastic simulation, noncontinuum models, kinetic Monte Carlo simulation, nonlinear control, gain-scheduled control, stochastic control, Markov processes

1. INTRODUCTION

The vast majority of the literature on feedback controller design is based on continuum models, which are described by systems of algebraic, ordinary differential, and partial differential equations (Levine, 1995). The continuum modeling approach, however, is inadequate for modeling much of the molecular and mesoscale phenomena that occur in the complex chemical processes that constitute the attention of today's scientists and engineers (Maroudas, 2000). This is especially apparent in microelectronics processes, for which the critical phenomena occur at the nanometer and smaller length scales. Hence in recent years increasing efforts have been directed towards the development of noncontinuum models, such as kinetic Monte Carlo (KMC) simulation models, for which most existing controller design techniques are not directly applicable. The design of feedback controllers based on such noncontinuum models is an open research problem in the field of control (Murray, 2002).

Global competition has increased the importance of feedback control for the complex chemical processes that are best described by noncontinuum models. There is probably no place where this is more apparent than in the microelectronics industry, which has had an average annual growth of 20%, with sales of $200 billion in 2001. It is generally accepted that high performance feedback control will be required to achieve the small length scales required to provide high computational speed in future microelectronic devices (Sematech, 2001).

Here feedback controllers are designed for a coupled KMC-finite difference (FD) code that simulates the electrochemical deposition of copper into a trench, a key step in the manufacturing on-chip interconnects for microelectronic devices (Andricacos, *et al.*, 1998). The industrial need is to deposit copper uniformly into trenches and vias of small dimension (less than 100 nm) under galvanostatic (constant current) conditions. This industrial importance has motivated numerous experimental and simulation studies on the modeling of copper electrodeposition

in recent years (Alkire and Eliadis, 1999; Andricacos, *et al.*, 1998; Georgiadou, *et al.*, 2001; Gill, 2001; Harper, *et al.*, 1999; Merchant, *et al.*, 2000; Moffet, *et al.*, 2000, Moffet, *et al.*, 2001). The goal of the feedback controller is to maintain the current (or current density) at a constant specified value. This feedback controller allows the KMC simulations to operate under industrial operating conditions.

The paper is organized as follows. First, the coupled KMC-FD copper electrodeposition simulation code is described. This is followed by construction of a low order stochastic model that is used to design feedback controllers and associated filters to handle the non-Gaussian stochastic noise produced by the KMC code. Then the closed-loop responses of the controllers are compared in simulations of the low order stochastic model and the KMC-FD simulation code.

2. COUPLED KINETIC MONTE CARLO-FINITE DIFFERENCE SIMULATION CODE

Kinetic Monte Carlo (KMC) methods are used to simulate structural properties of matter that cannot be represented by a macroscopic continuum description, and are widely used for simulating dynamic chemical and materials processes. A KMC simulation is a realization of the Master equation (Fichthorn and Weinberg, 1991):

$$\frac{\partial P(\sigma,t)}{\partial t} = \sum_{\sigma'} W(\sigma',\sigma)P(\sigma,t) - \sum_{\sigma'} W(\sigma,\sigma')P(\sigma,t) \tag{1}$$

where σ and σ' are successive states of the system, $P(\sigma, t)$ is the probability that the system is in state σ at time t, and $W(\sigma',\sigma)$ is the probability per unit time that the system will undergo a transition from state σ' to σ. For a particular system being studied, the KMC code chooses randomly among the possible transitions of the system and accepts particular transitions with appropriate probabilities. After each accepted or attempted transition, the time variable is incremented by one Monte Carlo time step, and the process is repeated. If the probabilities satisfy certain conditions, the real time variable t corresponding to the number of Monte Carlo time steps can be computed.

Electrochemical deposition of a copper film into a trench is simulated in this application. A KMC method was used since traditional continuum codes are not convenient for simulating the evolution of the roughness of the surface, which is an important characteristic of the produced copper film. The KMC code describes the mesoscale with a cubic lattice, where each subdomain in the simulation space represents a cluster of molecules (referred to as a mesoparticle) of a given species in the deposition bath (see Fig. 1). Each subdomain is cube of 12.5 nm on a side and is assumed to be homogeneous in both phase and composition. Similar mesoscale KMC methods have been applied by various researchers to a number of systems (Bird, 1994; Birdsall and, Langdon, 1985; Katsoulakis, *et al.*, 2002; Lu and Kushner, 2001). While molecular-scale simulations are of interest, this coarser mesoscale representation results in an efficient computational method that can simulate devices on the same scale as in the real system (Drews, *et al.*, 2003). The Monte Carlo simulation domain is a trench with aspect ratio 2:1, 40 subdomains wide, 80 subdomains high, and 6 subdomains deep.

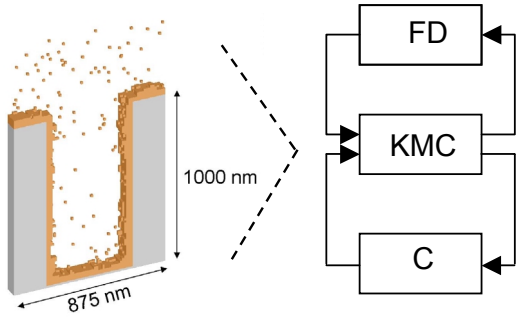

Fig. 1. Architecture of the KMC-FD simulation operating under feedback: FD denotes the finite difference code, KMC denotes the kinetic Monte Carlo code, and C denotes the controller. The KMC domain is on the left.

The kinetic Monte Carlo code simulates deposition phenomena by considering the likelihood of various actions that each mesoparticle can take at a given time step. These actions are bulk diffusion, surface diffusion, the reaction A→B, a combination reaction A+B→C, a splitting reaction A→B+C, and dissolution. All actions are computed as frequencies, with units of sec^{-1}. At a given Monte Carlo time step, a mesoparticle can make a maximum of one move. The possible moves that each species can make are a function of the location of the mesoparticle in the simulation space, as well as the number and type of the six nearest neighbors.

The Monte Carlo domain has periodic boundary conditions in the x and y directions, an impenetrable boundary at the electrode surface (in the z-direction), and a link to a continuum code at the top boundary in the z-direction. The continuum code is a one-dimensional FD code that provides diffusion fluxes of Cu^{2+} into the Monte Carlo domain by solving the diffusion equation. The KMC code provides the concentration of Cu^{2+} to the continuum code. The height of the continuum domain was set to 50 μm, which is close to the actual diffusion boundary layer

thickness that corresponds to typical processing conditions. In both the FD and KMC codes, an additive-free bath is simulated. The KMC code also produces a signal that is the charge passed during deposition, and reads as input the applied potential η. These signals serve as the input and output of the feedback controller (see Fig. 1).

Three time steps are tracked in the KMC simulation code: (1) the time step over which the continuum code is called for updated flux information, (2) the sampling interval for the feedback controller, and (3) the Monte Carlo (MC) time step. In order to capture the full dynamics of the system, the MC time step must be small enough to capture the action of the fastest species. For all the processes in this application, the Monte Carlo time step was computed to be ~2.8 μs. A complete KMC simulation run typically requires 1.08×10^8 MC time steps before the copper fills the trench. In this particular study, the linking time step and the sampling interval for the feedback controller are set to be 10^{-7} s and 10^{-2} s, respectively.

To carry out the galvanostatic (i.e., constant current) simulations associated with industrial operations, the feedback controller must manipulate the applied potential η to control the current i, based on the charge transferred as a function of time. There are two main performance requirements for the feedback controller. First, the feedback controller should have a tracking response as fast as possible. Second, 90% of the fluctuations in the applied potential should be within ±0.01 V. An additional requirement is for the controller to be low order, so that its computational cost is negligible compared to the cost of the KMC-FD calculations. The potential η enters the surface reaction frequencies in a nonlinear manner. This suggests that nonlinear control may give better performance than linear control. The next section describes how a low order stochastic model was constructed from input-output data collected from the KMC-FD code, and how this model was used to design feedback controllers.

3. IDENTIFICATION OF A LOW ORDER STOCHASTIC MODEL

The KMC-FD code is computationally expensive, highly stochastic, and nonlinear. To design low order feedback controllers, a low order stochastic model is constructed that is capable of capturing the most essential input-output behavior of the coupled KMC-FD code. This low order model is incorporated into model-based controller design and used for filter and controller tuning.

The output of the KMC-FD code is the cumulative charge passed up to current simulation time. To emulate the real physical system as closely as possible, the charge signal is converted to a current density signal. The current density was computed as the total charge passed in each 0.01 s, divided by 0.01 s and the surface area in cm^2. A larger time step interval could be used to compute the current from the charge, but this would lead to a more sluggish response, causing an inherent performance limitation in the feedback controller. On the other hand, decreasing the time step leads to more highly noise-corrupted signal. The manipulated variable is the applied potential, which affects the kinetics of the mechanisms simulated in the KMC-FD code and hence directly affects the current generation.

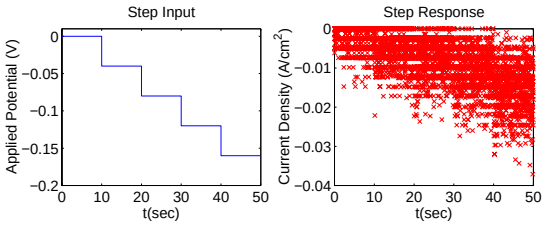

Fig. 2. Step input implemented on the KMC-FD code and the resulting step response.

The current density for a series of steps in the applied potential sent to the KMC-FD code is reported in Fig. 2. The applied potentials are selected to be within the normal operating condition of the KMC-FD simulation. Autocorrelations indicate that the current density reaches steady state within one sampling instance.

Upon reaching steady state, the output signal is bounded and its mean remains constant. These conditions justify the assumption that the signal is quasi-stationary (see Fig. 3). This assumption is verified by comparing the probability mass function of different time segments. The stochastic fluctuations are non-Gaussian and asymmetric, and can be modeled by a Poisson distribution for all normal operating conditions. To ensure consistency and accuracy, the identification procedure was repeated with different seed numbers. These sets of input-output data were used in the parameter estimation of a low order stochastic model:

$$P\big(i(k)=\kappa\,\big|\,\eta(k-1)\big)=\frac{\lambda^{-400\kappa}\exp(-\lambda)}{(-400\kappa)!} \qquad (2)$$

$$\lambda = 2.5285\exp(-6.5962\,\eta(k-1))-1.3622 \qquad (3)$$

where $\kappa\in\{-0.0025n,\, n\in \mathrm{Z}\}$ and Z is a set of non-negative integers. The form of the nonlinearity was motivated by the expression for the surface kinetics. Figure 3 compares the stochastic current density produced by the low order model (2)-(3) and the KMC-FD code for a range of applied potential.

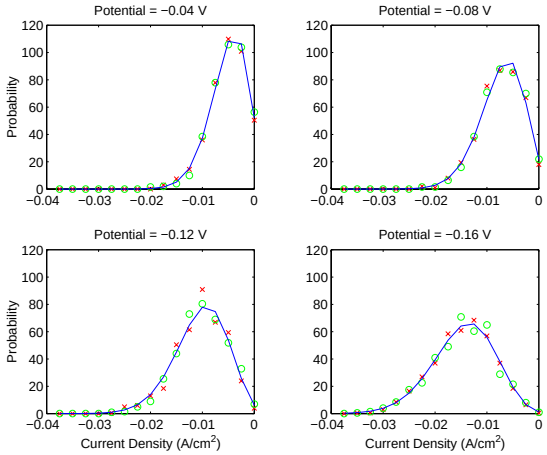

Fig. 3. Current density distributions for the low order model (solid line) and the KMC-FD code (× and o correspond to simulation data with different seed numbers).

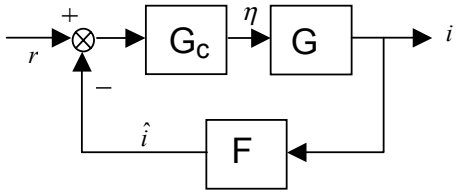

Fig. 4. Block diagram for the closed-loop system

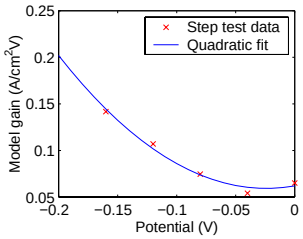

Fig. 5. Model gain of the KMC-FD code computed from step data.

4. FEEDBACK CONTROLLER DESIGN

Linear, gain-scheduled, and nonlinear inversion-based controllers were designed based on the low order stochastic model (2)-(3). Each controller incorporates a first-order filter (see Fig. 4):

$$F(z) = \frac{\alpha}{1-(1-\alpha)z^{-1}} \tag{4}$$

with filter constant α. This filter is used to reduce fluctuations in the manipulated variable without filtering the reference signal. The linear and nonlinear feedback controllers incorporate the deterministic part of the low order model (2)-(3):

$$i(k) = -6.3213\times10^{-3}\exp(-6.5962\,\eta(k-1)) + 3.4055\times10^{-3} \tag{5}$$

An alternative deterministic model used by the gain-schedule controller is to directly compute the model gain as a function of the manipulated variable (see Fig. 5). The model gain is computed based on the initial steady state condition at zero applied potential. The best least-squares quadratic fit to the model gain is:

$$K = 4.6058\,\eta^2 + 2.2074\times10^{-1}\,\eta + 6.1912\times10^{-2} \tag{6}$$

The two plant descriptions give almost the same output prediction.

4.1 Linear Controller

The range in system gain is given by

$$\{K \,|\, K \in \Re,\ 0.05 \le K \le 0.1417\} \tag{7}$$

where the upper bound was selected to exceed slightly the steady-state value for regulating the current density at –0.015 A/cm^2.

The linear feedback controller was designed using internal model control. Many other controller design techniques such as generic model control, direct synthesis, and geometric control give the same or similar control structures. The desired closed-loop response is first-order-plus-time-delay:

$$\frac{i}{r} = GG_c(1+FGG_c)^{-1} = \frac{(1-\exp(-\Delta t/\tau))z^{-1}}{1-\exp(-\Delta t/\tau)z^{-1}} \tag{8}$$

where τ is the desired closed loop time constant. This equation is rearranged to give the feedback controller

$$G_c = \frac{(1-\phi)-(1-\alpha)(1-\phi)z^{-1}}{1-(1+\phi(1-\alpha))z^{-1}+\phi(1-\alpha)z^{-2}}\cdot\frac{1}{K} \tag{9}$$

where $\phi = \exp(-\Delta t/\tau)$. Applying the small gain theorem to systems with time varying perturbations (Braatz and Morari, 1997) shows that choosing K = 0.1417 in the linear controller provides robustness for the full range of time-varying model gains in (7). The value τ = 10^{-5} s ensures fast response yet not faster than the dynamics of the KMC-FD simulation which is on the order of 10^{-6} s. The tuning of the filter constant α is discussed in Section 4.4.

4.2 Gain-scheduled Controller

The structure of the gain-scheduled controller is identical to the linear feedback controller. The only difference is that the gain K in (9) is updated at every time step using (6).

4.3 Nonlinear Controller

The nonlinear controller inserts an inverter derived from (5):

$$\eta(k) = -\frac{1}{6.5962}\ln\left(\frac{i(k) - 3.4055\times10^{-3}}{-6.3213\times10^{-3}}\right) \quad (10)$$

before the plant in the block diagram in Fig. 4. The plant combined with the inverter is a simple one-delay system that is controlled using the linear feedback controller with $K = 1$ in (9).

4.4 Filter Design

The filter constant α is tuned to ensure that at least 90% of the fluctuations in the applied potential are within ±0.01 V over the entire operating regime, while avoiding too much filtering which leads to unnecessarily sluggish response. The filter constant is designed based on the probability density distribution of the applied potential at the final time, that is, the time required to fill up the trench with copper. The reason for using the final time to design the filter coefficient is that the applied potential is the most negative at the final time, and the stochastic fluctuations are largest when the applied potential is the most negative. A filter coefficient that adequately filters the stochastic fluctuations at the final time also provides adequate filtering at earlier times.

A primary goal of this study was to create a filter and controller design procedure that can be quickly repeated when physicochemical parameters in the KMC-FD code are changed. Due to the high computational cost of running the KMC-FD code, its use in filter and controller design is limited to the creation of data for constructing the low order stochastic model (2)-(3). The low order model is then used to design the filter and controller. The probability density distribution of the applied potential at the final time was obtained by running the closed-loop simulation of the low order stochastic model 10,000 times at several α values. From this probability density distribution, the mean and the deviation corresponding to the 90% confidence level were estimated. Figure 6 shows how the deviation varies with the filter constant α. Table 1 reports the filter constants that result in 90% of the applied potential being within ±0.01 V at the final time.

Table 1. Filter constants for the three controllers

Controller type	α
Linear	0.03806
Gain-scheduled	0.03951
Nonlinear	0.03260

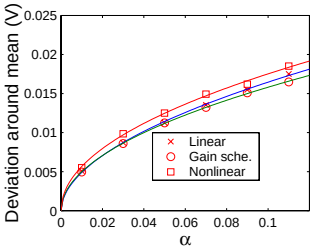

Fig. 6. The relationship between the filter constant α and the deviation around the mean at the final time corresponding to the 90% confidence level

5 RESULTS AND DISCUSSION

The controllers were implemented in the KMC-FD code and the low order stochastic model (2)-(3). Figure 7 shows agreement between the closed-loop predictions of the original and low order models. As specified, the applied potential is within ±0.01 V of its steady-state value 90% of the time, except for the initial transient.

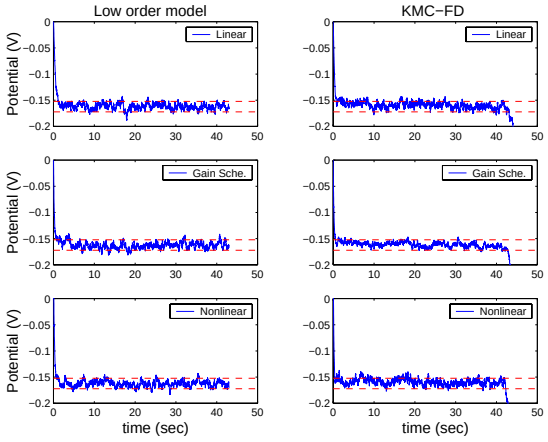

Fig. 7. Closed-loop responses for the linear, gain-scheduled, and nonlinear inversion-based controllers implemented on the low order model (2)-(3) and the KMC-FD code

Figures 8 and 9 focus on the initial time responses. The closed-loop performance is similar for the controllers, with the gain-scheduled controller slightly better than the others. Differences between the closed-loop simulations obtained with the low order stochastic model (2)-(3) and the KMC-FD code are within the stochastic variation in the responses. This is further support that use of the low order model for filter and controller design was justified. The applied potential in Fig. 8 reaches a quasi-steady-state value in ~0.5 s. Since the process dynamics are very fast, the unfiltered current density (not shown due to extremely large stochastic noise) reaches a quasi-state-value in ~0.5 s. The filtered current density, which includes the filter lag, reaches a quasi-steady-state value in 1 s.

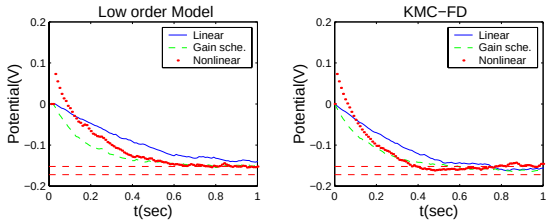

Fig. 8. The applied potentials for the three controllers implemented on the low order model (2)-(3) and the CED code

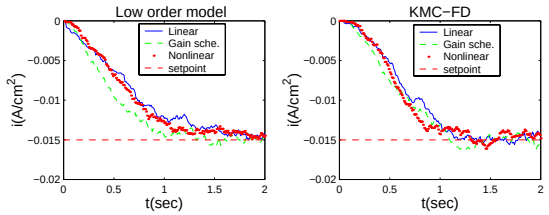

Fig. 9. The filtered current density for the three controllers implemented on the low order model (2)-(3) and the CED code

6. CONCLUSIONS

This paper demonstrates the design of low order linear, nonlinear, and gain-scheduled feedback controllers for a coupled kinetic Monte Carlo-finite difference code that simulates infill of a trench during copper electrodeposition. The feedback controllers and associated filters were constructed from a low order stochastic model constructed from data collected from the KMC-FD code. The controllers enable the KMC-FD code to operate with nearly constant current, which is the industrial operating condition.

7. ACKNOWLEDGEMENTS

The authors gratefully acknowledge support from the National Science Foundation (CTS-0135621, NRAC-MCA01S022). Any opinions, findings, conclusions, or recommendations expressed in this paper are those of the authors and do not necessarily reflect the views of the National Science Foundation.

8. REFERENCES

Alkire, R.C., and E.D. Eliadis (1999). Electro-deposition of copper: The effect of various organic compounds. *Z. Phys. Chem.*, **208**, 1-15.

Andricacos, P.C., C. Uzoh, J.O. Dukovic, J. Horkins, and H. Deligianni (1998). Damascene copper electroplating for chip interconnections. *IBM J. Res. Dev.*, **42**, 567-574.

Bird, G.A. (1994). *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon Press, Oxford.

Birdsall, C.K. and A.B. Langdon (1985). *Plasma Physics via Computer Simulation*. McGraw-Hill, New York.

Braatz, R.D. and M. Morari (1997). A multivariable stability margin for systems with mixed time-varying parameters. *Int. J. of Robust and Nonlinear Control*, **7**, 105-112.

Drews, T.O., R.D. Braatz, and R.C. Alkire (2003). Parameter sensitivity analysis of Monte Carlo simulations of copper electrodeposition with multiple additives. *J. Electrochem. Soc.* accepted.

Fichthorn, K.A. and W.H. Weinberg (1991). Theoretical foundations of dynamic Monte-Carlo simulations. *J. Chem. Phys.*, **95**, 1090-1096.

Georgiadou, M., D. Veyret, R.L. Sani, and R.C. Alkire (2001). Simulation of shape evolution during electrodeposition of copper in the presence of additive. *J. Electrochem. Soc.*, **148**, C54-C58.

Gill, W.N., D.J. Duquette, and D. Varadarajan (2001). Mass transfer models for the electrodeposition of copper with a buffering agent. *J. Electrochem. Soc.*, **148**, C289-C296.

Harper, J.M.E., C. Cabral, P.C. Andricacos, L. Gignac, I.C. Noyan, K.P. Rodbell, and C.K. Hu (1999). Mechanisms for microstructure evolution in electroplated copper thin films near room temperature. *J. Appl. Phys.*, **86**, 2516-2525.

Katsoulakis, M.A., A.J. Majda, and D.G. Vlachos (2002). Course-grained stochastic processes and Monte Carlo simulations in lattice systems. Univ. of Delaware, Newark. Technical report.

Levine, W.S., ed. (1995). *The Control Handbook*. CRC Press, Boca Raton, FL.

Lu, J., and M.J. Kushner. Trench filling by ionized metal physical vapor deposition (2001). *J. Vac. Sci. Technol. A*, **19**, 2652-2663.

Maroudos, D. (2000). Multiscale modeling of hard materials: Challenges and opportunities for chemical engineering. *AIChE J.*, **46**, 878.

Merchant, T.P., M.K. Gobbert, T.S. Cale, and L.J. Borucki (2000). Multiple scale integrated modeling of deposition processes. *Thin Solid Films*, **365**, 368-375.

Moffet, T.P., J.E. Bonevich, W.H. Huber, A. Stanishevsky, D.R. Kelly, G.R. Stafford, and D. Josell (2000). Superconformal electrodepositon of copper in 500-90 nm features. *J. Electrochem. Soc.*, **147**, 4524-4535.

Moffet, T.P., D. Wheeler, W.H. Huber, and D. Josell (2001). Superconformal electrodeposition of copper. *Electrochem. Solid State*, **4**, C26-C29.

Murray, R. M., ed. (2003). *Control in an Information Rich World*, SIAM Press, Philadelphia, PA.

Sematech (2001). International Technology Roadmap for Semiconductors, Semiconductor Industry Association, http://public.itrs.net/.