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NUMERICAL METHOD FOR COMPUTER MODELING OF DIFFUSION OF IMPLANTED DOPANT ATOMS IN SILICON IN MODERN VLSI TECHNOLOGY

An extended five-stream model for diffusion in silicon is presented. A finite-difference method for computer modeling of dopant diffusion during post-implantation annealing is developed. Conservative implicit finite-difference schemes are obtained using integration-interpolation method. The nonlinear algebraic equation describing the local electroneutrality condition is solved using the bisection method. The obtained nonlinear system of difference equations is solved by iterative method.

Introduction

The mainstream in modern VLSI technology is further miniaturization. Of particular importance is decreasing the depth of p - n junctions in transistors down to nanometric size, which permits improving their working parameters and minimizing the so-called short-channel effect (leakage from drain to source when the transistor is off). The ultrashallow p - n junctions (USJ) in modern VLSI technology are produced by high-dose ion implantation of donor (As , P , Sb) or acceptor (e.g., B) dopants into a silicon wafer. The energy of ions is ~ 1 – 10 keV; this is the so-called low-energy implantation as opposed to the high-energy technology (~ 1 – 0.1 MeV) used in the previous generation of VLSI chips. After implantation, rapid thermal annealing (RTA) is used to heal the defects generated by implantation and perform the so-called electrical activation of the dopant atoms. However, during RTA, as well as during other kinds of post-implantation thermal treatment (e.g., spike annealing), the phenomenon of transient enhanced diffusion (TED) is observed: the apparent diffusion coefficient of the impurity atoms increases by several orders of magnitude, and near the outer surface uphill diffusion takes place [1–3]. This complex phenomenon is currently a subject of extensive experimental investigation because it hampers obtaining an optimal concentration profile of the dopants and hence hinders attaining the required current-voltage characteristics of transistors in VLSI circuits [1, 2].

TED is typically ascribed to the interaction of diffusing species with non-equilibrium point defects (vacancies V and silicon self-interstitials I), which are accumulated in silicon due to ion damage. Solving the intricate problem of TED suppression is impossible without mathematical modeling of this complex phenomenon. However, modern technology computer-aided design (TCAD) software packages such as SUPREM-IV by Silvaco Data Systems encounter severe difficulties in predicting TED of implanted dopants. Therefore, development of novel models to provide a correct physical description of TED is an urgent problem in the VLSI technology. Most of the models used in this area, including those implemented in popular package SUPREM-IV, employ the so-called five-stream approach [4–6], which was first put forward in Ref. [7]. In crystalline silicon, diffusion of dopant atoms can proceed via pairs "dopant atom-vacancy" AV and "dopant atom-silicon self-interstitial" AI , which can have several charge states $(AI)^\alpha$, $(AV)^\alpha$, $\alpha=0, \pm 1$ [8]. Also, the diffusion of free point defects $X=V, I$, which exist in multiple charge states X^γ , $\gamma=0, \pm 1, \pm 2$, takes place [4–7] and is accompanied by interaction between dissimilar diffusing species (generation and recombination of pairs). Recently, an extended five-stream model has been developed, which takes into account all the possible charge states of the diffusing species and the kinetics of interaction between them [9, 10].

In connection with the above, the goal of this work is the development of an efficient numerical method to solve a set of nonlinear partial differential equations, which describe the reaction-diffusion processes in silicon during RTA, for calculating the concentration profile of dopant atoms in the transistor and predicting the current-voltage characteristics of the latter.

Formulation of the mathematical model

In this work, we consider one-dimensional diffusion of an acceptor impurity, viz. boron (B); hence the free charge carriers in boron-doped silicon are positively charged holes. The model consists of four partial differential reaction-diffusion equations for diffusing pairs AV and AI ($A=B$) and point defects I and V , which account for the effect of built-in electric field on the diffusion of differently charged species and include the sink/source terms describing the interaction of dissimilar species (in particular, the formation and recombination of pairs AI and AV and annihilation of non-equilibrium point defects):

$$\frac{\partial C_I}{\partial t} = \frac{\partial}{\partial x} \left[D_I \frac{\partial C_I}{\partial x} + D_{I,p}(C_I, p) \frac{\partial}{\partial x} \left(\frac{p}{n_i} \right) \right] - R_{I-V}(C_I, C_V, p) - R_{A-I}(C_A, C_I, C_{AI}, p) - R_{AV-I}(C_{AV}, C_I, C_A, p), \quad (1)$$

$$\frac{\partial C_V}{\partial t} = \frac{\partial}{\partial x} \left[D_V \frac{\partial C_V}{\partial x} + D_{V,p}(C_V, p) \frac{\partial}{\partial x} \left(\frac{p}{n_i} \right) \right] - R_{I-V}(C_I, C_V, p) - R_{A-V}(C_A, C_V, C_{AV}, p) - R_{AV-V}(C_{AV}, C_V, C_A, p). \quad (2)$$

$$\frac{\partial C_{AI}}{\partial t} = \frac{\partial}{\partial x} \left[D_{AI}(C_I, p) \frac{\partial C_{AI}}{\partial x} + D_{AI,p}(C_I, C_{AI}, p) \frac{\partial}{\partial x} \left(\frac{p}{n_i} \right) \right] + R_{A-I}(C_A, C_I, C_{AI}, p) - R_{AI-V}(C_{AI}, C_I, C_A, p) - R_{AV-AI}(C_{AV}, C_{AI}, C_A, p), \quad (3)$$

$$\frac{\partial C_{AV}}{\partial t} = \frac{\partial}{\partial x} \left[D_{AV}(C_V, p) \frac{\partial C_{AV}}{\partial x} + D_{AV,p}(C_V, C_{AV}, p) \frac{\partial}{\partial x} \left(\frac{p}{n_i} \right) \right] + R_{A-V}(C_A, C_V, C_{AV}, p) - R_{AV-I}(C_{AV}, C_I, C_A, p) - R_{AV-AV}(C_{AV}, C_{AV}, C_A, p). \quad (4)$$

Besides, there are two additional equations: a differential equation for the evolution of the charged, i.e. electrically active dopant atoms (here boron) in the lattice sites

$$\frac{\partial C_A}{\partial t} = R_{AI-V}(C_{AI}, C_V, C_A, p) + R_{AV-I}(C_{AV}, C_I, C_A, p) + 2R_{AV-AV}(C_{AV}, C_{AV}, C_A, p) - R_{A-I}(C_A, C_I, C_{AI}, p) - R_{A-V}(C_A, C_V, C_{AV}, p), \quad (5)$$

and the nonlinear algebraic equation describing the condition of local electroneutrality (because the mobility of holes is much higher than that of charged diffusing species):

$$\beta C_A + \sum_{\alpha=\pm 1} \alpha C_{I,AY}(C_{AY}, p) + \sum_{\alpha=\pm 1} \alpha C_{I,AV}(C_{AV}, p) + \sum_{\gamma=\pm 1, \pm 2} \gamma C_I(C_I, p) + \sum_{\gamma=\pm 1, \pm 2} \gamma C_V(C_V, p) + p - n_i^2 / p = 0. \quad (6)$$

Here $C_Y, Y \equiv I, V, AI, AV$, are the volumetric concentrations of diffusing species (point defects and pairs), which are defined as a sum over all the possible charge states: $C_Y = \sum_{\alpha} C_{Y^{\alpha}}$, where $\alpha=0, \pm 1$ for pairs AI and AV ,

$\alpha=0, \pm 1, \pm 2$ for point defects; C_A is the concentration of dopant atoms (B) in the lattice sites; p is the concentration of holes; D_Y is the diffusion coefficient of corresponding species. D_I and D_V being constant at a given temperature; $D_{Y,p}$ is the electrodiffusion coefficient describing the effect of a built-in electric field, which arises due to non-uniform distribution of free charge carriers (here holes) in the doped silicon crystal, on the diffusion of charged species; $R_{Y-Z}, Y, Z \equiv I, V, A, AI, AV, Y \neq Z$, are the reaction-rate terms describing the interaction between dissimilar species; α and γ are the charges of pairs and point defects, correspondingly; β is the charge of dopant atoms in the lattice sites, $\beta = -1$ for acceptors (because here $A \equiv B$); n_i is the intrinsic concentration of free charge carriers (here electrons), which is known in literature and depends only on temperature.

The free outer surface (at $x=0$) of crystalline silicon is a natural sink for point defects. Thus, equilibrium concentration of the latter is always sustained there, while for diffusion of pairs the mirror-like, or Neumann boundary conditions should be imposed at $x=0$. Similar conditions hold true at $x \rightarrow \infty$. Then the boundary conditions in the domain $x \in [0, l]$, where l is the maximal diffusion depth, are formulated as follows:

$$C_I|_{x=0} = C_I|_{x=l} = C_I^*, \quad (7)$$

$$C_V|_{x=0} = C_V|_{x=l} = C_V^*, \quad (8)$$

$$J_{AI}|_{x=0, x=l} = - \left[D_{AI}(C_I, p) \frac{\partial C_{AI}}{\partial x} + D_{AI,p}(C_I, C_{AI}, p) \frac{\partial}{\partial x} \left(\frac{p}{n_i} \right) \right]_{x=0, x=l} = 0, \quad (9)$$

$$J_{AV} \Big|_{x=0, x=l} = - \left[D_{AV} (C_V, p) \frac{\partial C_{AV}}{\partial x} + D_{AV/p} (C_V, C_{AI}, p) \frac{\partial}{\partial x} \left(\frac{p}{n_e} \right) \right]_{x=0, x=l} = 0, \quad (10)$$

where C_i^* and C_V^* are the equilibrium concentrations of point defects at a given temperature, J is the diffusion flux.

The initial conditions (concentration profiles of point defects, lattice atoms A and pairs AI , AV at $t=0$) to reaction-diffusion equations (1)–(5) depend on the implantation conditions and are determined by Monte Carlo simulation [11, 12].

Finite-difference approximation

For performing numerical solution of the formulated problem, the finite difference method is used. In domain Ω , a discrete grid $\omega_x \times \omega_t$ is introduced so that

$$\omega_x = \{x_i = ih, h > 0, i = 0, 1, \dots, N, Nh = l\}, \omega_t = \{t_j = j\tau, \tau > 0, j = 0, 1, \dots, M, M\tau = T\}, \quad (11)$$

where h is a step over axis $0x$ and τ is a temporal step.

For any function defined on the grid, $y(x, t_j)$, the finite-difference derivatives are determined as follows: $y_x = (y'_{i+1} - y'_i) / h$, $i = 0, 1, \dots, N-1$, $j = 0, 1, \dots, M$ (a forward derivative), $y_x = (y'_i - y'_{i-1}) / h$, $i = 1, 2, \dots, N$, $j = 0, 1, \dots, M$ (a backward derivative), and $y_t = (y'_i - y'_{i-1}) / \tau$, $i = 0, 1, \dots, N-1$, $j = 1, 2, \dots, M$ (a time derivative). The discrete (i.e. approximate) values of variables C_b , C_i , C_{AI} , C_{AV} , C_b , p on the finite grid are denoted as y_1, y_2, \dots, y_6 , correspondingly.

To construct conservative finite-difference schemes for partial differential equations (1)–(4), we employ the universal integration-interpolation method [13]: the equations are integrated over the cell $[x_{i-1/2}, x_{i+1/2}] \times [t_{j-1}, t_j]$, $i = 1, \dots, N-1$, $j = 1, 2, \dots, M$. After that the integrals are approximated by linear combinations of variables y_k , $k = 1, 6$ and relevant coefficients in the corresponding lattice nodes. The resulting systems of non-linear finite-difference equations look as

$$y_{1,i} = [D_I y_{1,x} + a_1(y_1, y_6) y_{6,\tau}]_x - R_{I-A}(y_1, y_2, y_6) - R_{I-V}(y_5, y_1, y_3, y_6) - R_{AV-I}(y_4, y_1, y_5, y_6), \quad i = 1, 2, \dots, N-1, \quad j = 1, 2, \dots, M, \quad (12)$$

$$y_{2,j} = [D_V y_{2,x} + a_2(y_2, y_6) y_{6,\tau}]_x - R_{I-V}(y_1, y_2, y_6) - R_{AV-V}(y_5, y_2, y_4, y_6) - R_{AI-V}(y_3, y_2, y_5, y_6), \quad i = 1, 2, \dots, N-1, \quad j = 1, 2, \dots, M, \quad (13)$$

$$y_{3,i} = [a_3(y_1, y_6) y_{1,x} + a_4(y_1, y_3, y_6) y_{6,\tau}]_x + R_{A-I}(y_5, y_1, y_3, y_6) - R_{AI-V}(y_1, y_2, y_5, y_6) - R_{AI-AI}(y_4, y_1, y_5, y_6), \quad i = 1, 2, \dots, N-1, \quad j = 1, 2, \dots, M, \quad (14)$$

$$y_{4,i} = [a_5(y_2, y_6) y_{4,x} + a_6(y_2, y_4, y_6) y_{6,\tau}]_x + R_{A-I}(y_5, y_2, y_4, y_6) - R_{AV-V}(y_4, y_1, y_5, y_6) - R_{AV-AI}(y_4, y_3, y_5, y_6), \quad i = 1, 2, \dots, N-1, \quad j = 1, 2, \dots, M, \quad (15)$$

$$y_{5,j} = R_{AI-V}(y_3, y_2, y_5, y_6) + R_{AV-I}(y_4, y_1, y_5, y_6) + 2R_{AI-AI}(y_4, y_1, y_5, y_6) - R_{A-I}(y_5, y_1, y_6) - R_{AV-V}(y_5, y_2, y_4, y_6), \quad i = 0, 1, \dots, N, \quad j = 1, 2, \dots, M, \quad (16)$$

$$-y_5 + \sum_{\alpha=\pm 1} \alpha C_{(AI)V}(y_1, y_6) + \sum_{\alpha=\pm 1} \alpha C_{(AI)V}(y_4, y_6) + \sum_{\alpha=\pm 1, \pm 2} \gamma C_{I^*}(y_1, y_6) + \sum_{\gamma=\pm 1, \pm 2} \gamma C_{I^*}(y_2, y_6) + y_6 - n_e^2 / y_6 = 0, \quad i = 0, 1, \dots, N, \quad j = 1, 2, \dots, M. \quad (17)$$

Here parameters a_1, a_2, \dots, a_6 are determined as follows:

$$\begin{aligned} a_1(y_1, y_6) &= 0.5[D_{Iip}(y_{1,i}, y_{6,i}) + D_{Iip}(y_{1,i-1}, y_{6,i-1})], \\ a_2(y_2, y_6) &= 0.5[D_{Vip}(y_{2,i}, y_{6,i}) + D_{Vip}(y_{2,i-1}, y_{6,i-1})], \\ a_3(y_1, y_6) &= 0.5[D_{AI}(y_{1,i}, y_{6,i}) + D_{AI}(y_{1,i-1}, y_{6,i-1})], \\ a_4(y_1, y_3, y_6) &= 0.5[D_{AIip}(y_{1,i}, y_{3,i}, y_{6,i}) + D_{AIip}(y_{1,i-1}, y_{3,i-1}, y_{6,i-1})], \\ a_5(y_2, y_6) &= 0.5[D_{AV}(y_{2,i}, y_{6,i}) + D_{AV}(y_{2,i-1}, y_{6,i-1})], \end{aligned} \quad (18)$$

$$a_6(y_2, y_4, y_6) = 0.5[D_{AVP}(y_{2i}, y_{4i}, y_{6i}) + D_{AVP}(y_{2i-1}, y_{4i-1}, y_{6i-1})], \quad i=1, 2, \dots, N,$$

where subscript i denotes the number of node along the $0x$ axis.

The boundary conditions (7), (8) look as

$$y_1|_{i=0} = y_1|_{i=N} = C_1^*, \quad y_2|_{i=0} = y_2|_{i=N} = C_2^*, \quad (19)$$

while boundary conditions (9), (10) are approximated using the Taylor series expansion:

$$0.5\delta h[y_{3i} - R_{i-1}(y_3, y_1, y_3, y_6) + R_{i+1}(y_3, y_2, y_5, y_6) + R_{i-1}(y_4, y_3, y_3, y_6)]_{i=0, N} = [a_3(y_1, y_6)y_{3\tau} + a_4(y_1, y_3, y_6)y_{6\tau}]_{i=0, N}, \quad (20)$$

$$0.5\delta h[y_{4i} - R_{i-1}(y_3, y_2, y_4, y_6) + R_{i+1}(y_4, y_1, y_5, y_6) + R_{i-1}(y_4, y_3, y_3, y_6)]_{i=0, N} = [a_5(y_2, y_6)y_{4\tau} + a_6(y_2, y_4, y_6)y_{6\tau}]_{i=0, N}, \quad (21)$$

where $\delta = 1$ for $i=0$, $\delta = -1$ for $i=N$.

Since the discrete equations (12)–(17), (20) and (21) are nonlinear, the numerical solution of the problem under consideration can be found using an iteration procedure which is described below.

Iteration procedure

The system of finite-difference equations (12) – (16) together with boundary conditions (19)–(21) and discrete algebraic equation (17) is linearized in the following manner:

$$y_{1i}^{s+1} = [D_1 y_{1\tau}^{s+1} + a_1(y_1^s, y_6^s)y_{6\tau}^s]_i - R_{i-1}(y_1^s, y_2^s, y_6^s) - R_{i+1}(y_5^s, y_1^s, y_3^s, y_6^s) - R_{i-1}(y_4, y_1, y_3, y_6)^s, \quad (22)$$

$$y_{2i}^{s+1} = [D_2 y_{2\tau}^{s+1} + a_5(y_2^s, y_6^s)y_{6\tau}^s]_i - R_{i-1}(y_1^s, y_2^s, y_6^s) - R_{i+1}(y_3^s, y_2^s, y_4^s, y_6^s) - R_{i-1}(y_3, y_2, y_5, y_6)^s, \quad (23)$$

$$y_{3i}^{s+1} = [a_3(y_1^s, y_6^s)y_{3\tau}^s + a_4(y_1^s, y_3^s, y_6^s)y_{6\tau}^s]_i + R_{i-1}(y_3^s, y_1^s, y_3^s, y_6^s) - R_{i+1}(y_3, y_2, y_5, y_6)^s - R_{i-1}(y_4, y_3, y_3, y_6)^s, \quad (24)$$

$$y_{4i}^{s+1} = [a_5(y_2^s, y_6^s)y_{4\tau}^s + a_6(y_2^s, y_4^s, y_6^s)y_{6\tau}^s]_i + R_{i-1}(y_3^s, y_2^s, y_4^s, y_6^s) - R_{i+1}(y_4, y_1, y_5, y_6)^s - R_{i-1}(y_4, y_3, y_3, y_6)^s, \quad (25)$$

$$y_{5i}^{s+1} = R_{i-1}(y_3^s, y_2^s, y_5^s, y_6^s) + R_{i+1}(y_3, y_1, y_3, y_6)^s - R_{i-1}(y_5, y_1, y_3, y_6)^s + 2R_{i-1}(y_4, y_3, y_5, y_6)^s - R_{i-1}(y_5, y_2, y_4, y_6)^s, \quad (26)$$

$$-y_5^{s+1} + \sum_{\alpha=\pm 1} \alpha C_{(1)\tau}^{s+1}(y_3^s, y_6^s) + \sum_{\alpha=\pm 1} \alpha C_{(1)\tau}^{s+1}(y_4^s, y_6^s) + \sum_{\gamma=\pm 1, \pm 2} \gamma C_{\tau}^{s+1}(y_1^s, y_6^s) + \sum_{\gamma=\pm 1, \pm 2} \gamma C_{\tau}^{s+1}(y_2^s, y_6^s) + y_6^{s+1} - n_0^2/y_6^{s+1} = 0, \quad (27)$$

$$y_1|_{i=0}^{s+1} = y_1|_{i=N}^{s+1} = C_1^*, \quad y_2|_{i=0}^{s+1} = y_2|_{i=N}^{s+1} = C_2^* \quad (28)$$

$$0.5\delta h[y_{3i} - R_{i-1}(y_3, y_1, y_3, y_6) + R_{i+1}(y_3, y_2, y_5, y_6) + R_{i-1}(y_4, y_3, y_3, y_6)]_{i=0, N} = [a_3(y_1, y_6)y_{3\tau} + a_4(y_1, y_3, y_6)y_{6\tau}]_{i=0, N}, \quad (29)$$

$$0.5\delta h [y_{4,j}^{s+1} - R_{A-V}(y_4^s, y_2^s, y_4^s, y_6^s) + R_{V-I}(y_4^s, y_1^s, y_5^s, y_6^s) + R_{A-V-I}(y_4^s, y_3^s, y_5^s, y_6^s)]_{i=0,N} = [a_5(y_2^s, y_6^s) y_{4,\tau}^{s+1} + a_6(y_2^s, y_4^s, y_6^s) y_{6,\tau}^{s+1}]_{i=1,N}, \quad (30)$$

where s and $s+1$ are the iteration numbers; Eqs. (22)–(26) refer to nodes $i=1,2,\dots,N-1, j=1,2,\dots,M$ and Eq.(27) refers to all the nodes: $i=0,1,\dots,N, j=1,2,\dots,M$; in Eqs.(29), (30) $\delta = 1$ for $i=0$, $\delta = -1$ for $i=N$. Here the following notation is used:

$$y_K \equiv y_{K,i}^s, \quad y_K \equiv y_{K,i}^{s+1}, \quad y_{K,j} \equiv \left(y_{K,i}^s - y_{K,i}^{s+1} \right) / \tau, \quad K = \overline{1,6}, \quad i=0,1,\dots,N, j=1,2,\dots,M,$$

where subscript K is the number of a variable and superscripts $j, j-1$ denote the number of a temporal layer.

For the zero iteration, the values on a previous temporal layer are taken:

$$y_{K,i}^{j=0} = y_{K,i}^{j-1}, \quad K = \overline{1,6}, \quad i=0,1,\dots,N. \quad (31)$$

The system of fully implicit finite-difference equations (22)–(25) with boundary conditions (28)–(30) is solved for $y_K^{s+1}, K = \overline{1,5}$, using the economical Thompson method; Eq. (26) is an algebraic one and is solved directly for the unknown values of y_5^{s+1} ; nonlinear algebraic equation (27) is solved numerically for y_6^{s+1} by the bisection method which provides unconditional convergence. The iterations are continued until convergence of the numerical solution is attained, i.e. the following condition is satisfied:

$$|y_{K,i}^{s+1} - y_{K,i}^s| < \varepsilon_1 |y_{K,i}^{s+1}| + \varepsilon_2, \quad K = \overline{1,6}, \quad i = 0,1,2,\dots,N, \quad (32)$$

where ε_1 and ε_2 are the prescribed tolerances (empirical parameters).

Conclusion

Thus, a finite-difference method and algorithm is developed for solving a system of nonlinear partial-differential equations that describe the diffusion of boron atoms in monocrystalline silicon during post-implantation annealing. Basing on the algorithm, a computer code is elaborated which can be used for modeling of diffusion of implanted dopants in silicon during the production of ultrashallow $p-n$ junctions in VLSI circuits. Computer modeling using this code will permit decreasing the undesirable TED phenomenon, predicting the dopant distribution in a transistor and current-voltage characteristic of the latter, and optimizing the parameters of implantation and subsequent thermal annealing in modern VLSI technology.

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SECURE SHELL SESSION RESUMPTION

The Secure Shell (SSH) Protocol is a protocol for secure remote login and other secure network services over an insecure network. However, using modern cryptography techniques might be computationally expensive, especially for low-end devices such as wireless access points and DSL routers. Here I present an implementation of a session resumption mechanism that has been proposed earlier to improve the performance of SSH.

Introduction

Secure Shell is a network protocol that allows data to be exchanged using a secure channel between two networked devices. The encryption used by SSH provides confidentiality and integrity of data over an insecure network, such as the Internet. Symmetric-key encryption algorithms are used by SSH, so both a decryption and an encryption are accomplished by identical cryptographic keys. Therefore before starting an encrypted session SSH uses some mechanisms that allows two parties that have no prior knowledge of each other to establish a shared secret key over an insecure communications channel. But the modern cryptography techniques that are used to accomplish this are very computationally expensive. A key exchange procedure takes place only once during the initial phase of the SSH connection. Nevertheless the performance can be significantly affected when new connections are repeatedly established over a short period of time, especially in case of devices with limited resources.

A session resumption mechanism allows to use the session key from the previous connection, instead of establishing a new one, thus it avoids a costly key computation procedure.

Secure Shell protocol

Secure Shell (SSH) protocol consists of three major components: Transport Layer Protocol, User Authentication Protocol and Connection Protocol.

Transport Layer Protocol defined in the RFC4253 [2] provides server authentication, confidentiality, and integrity. It may optionally also provide compression. Typically the transport layer is run over a TCP/IP connection.

The User Authentication Protocol defined in the RFC4252 [3] authenticates the client-side user to the server and it runs over the transport layer protocol.